PB84-210939

Air Quality Models Pertaining to Particulate Matter

Massachusetts Inst. of Tech., Cambridge
Energy Lab.

Prepared for

Environmental Sciences Research Lab.
Research Triangle Park, NC

Jun 84

U.S. Department of Commerce
National Technical Information Service
NTIS

PB84-210939

EPA-600/3-84 074
June 1984

AIR QUALITY MODELS PERTAINING TO PARTICULATE MATTER

by

S.A. Batterman, J.A. Fay, D. Golomb, J. Gruhl
Energy Laboratory
Massachusetts Institute of Technology
Cambridge, MA 02139

Cooperative Agreement Number 809229-01

Project Officer

Jack H. Shreffler
Meteorology and Assessment Division
Environmental Sciences Research Laboratory
Research Triangle Park, NC 27711

ENVIRONMENTAL SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA-600/3-84-074		PB84 210939

4. TITLE AND SUBTITLE	5. REPORT DATE
Air Quality Models Pertaining to Particulate Matter	June 1984
	6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
S.A. Batterman, J.A. Fay, D. Golomb, J. Gruhl	

9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT NO.
Energy Laboratory Massachusetts Institute of Technology Cambridge, MA 02139	CDTA1D/02 - 3156 (FY-84)
	11. CONTRACT/GRANT NO. Cooperative Agreement 809229-01

12. SPONSORING AGENCY NAME AND ADDRESS	13. TYPE OF REPORT AND PERIOD COVERED
Environmental Sciences Research Laboratory - RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, NC 27711	Final 04/83 - 10/88
	14. SPONSORING AGENCY CODE EPA/600/09

15. SUPPLEMENTARY NOTES

16. ABSTRACT This report describes an evaluation of the Particle Episodic Model (PEM), an urban scale dispersion model which incorporates deposition, gravitational settling and linear transformation processes into the predecessor model, the Texas Episodic Model (TEM-8). A sensitivity analysis of the model was performed, which included the effects of deposition, gravitational settling and receptor grid size. Recommendations are made to improve the performance and flexibility of the model.

PEM was applied to a source inventory of the Philadelphia area to provide a preliminary estimate of source apportionment. PEM modeling employed both hypothetical and actual meteorology. Results indicate that area source emissions dominate TSP, SO_2 and sulfate concentrations at urban receptors. A large fraction of the inhalable particles may arrive from distant sources.

This report also contains an overview of receptor models (RMs) used for the source apportionment of aerosols. Some diagnostic procedures for RMs are evaluated using a synthetic data set. Described are RM trade-offs and protocols and possible hybrid dispersion/receptor models. Issues regarding the inter-comparison of source apportionments from receptor and dispersion models are highlighted with reference to the 1982 Philadelphia study.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	82
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

ABSTRACT

This report describes an evaluation of the Particle Episodic Model (PEM), an urban scale dispersion model which incorporates deposition, gravitational settling and linear transformation processes into the predecessor model, the Texas Episodic Model (TEM-8). A sensitivity analysis of the model was performed, which included the effects of deposition, gravitational settling and receptor grid size. Recommendations are made to improve the performance and flexibility of the model.

PEM was applied to a source inventory of the Philadelphia area to provide a preliminary estimate of source apportionment. PEM modeling employed both hypothetical and actual meteorology. Results indicate that area source emissions dominate TSP, SO_2 and sulfate concentrations at urban receptors. A large fraction of the inhalable particles may arrive from distant sources.

This report also contains an overview of receptor models (RMs) used for the source apportionment of aerosols. Some diagnostic procedures for RMs are evaluated using a synthetic data set. Described are RM trade-offs and protocols and possible hybrid dispersion/receptor models. Issues regarding the inter-comparison of source apportionments from receptor and dispersion models are highlighted with reference to the 1982 Philadelphia study.

This report was submitted in fulfillment of Cooperative Agreement Number 809229-01 by the M.I.T. Energy Laboratory under the sponsorship of the U.S. Environmental Protection Agency. This report covers a period from April to October 1983 and work was completed as of November 4, 1983.

ACKNOWLEDGEMENTS

The authors appreciate the guidance and assistance offered by the Project Officers, Drs. K. Demerjian and J. Shreffler, and the comments, discussion and data provided by Drs. R. Stevens, T. Dzubay, C. Lewis and the scientists and engineers of the environmental agencies of the City of Philadelphia and the States of New Jersey and Pennsylvania.

CONTENTS

Abstract iii
Figures vi
Tables vii

1. Introduction 1

2. Conclusions and Recommendations 3

3. Evaluation of Particle Episodic Model 5
PEM Verification 5
Transferral and Compilation 5
Comparison to TEM-8 6
Deposition and Settling 6
Transformation 10
Area Sources 11
PEM Improvements 16
Deposition, Settling and Transformation 16
Source Specifications 18
Area Sources 19
Outputs 18
Miscellaneous 19
Summary 21

4. Source Apportionment Using PEM 22
Philadelphia Source Inventory 22
Meteorology 29
Dispersion Modeling 29
Hypothetical Meteorology 30
Actual Meteorology 35
Discussion 40

5. Receptor Models 43
Overview of Receptor Models 43
Chemical Mass Balance Receptor Models 45
Multivariate Receptor Models 47
Composite Receptor Models 47
Diagnostic Procedures for CMB Models 48
Collinearity 48
Source Selection 51
Influential Characteristics 53
Robust Regression 60
Hybrid Receptor/Dispersion Models 61
Comparisons Between Source and Receptor Models 64
Evaluative Criteria 64
Averaging Time 65
Receptor Model Protocols 67
Protocols for Monitoring and Analysis 68
Modeling Protocols 69
Protocols for Inter-Comparison of Receptor Models . 70
Summary 70

References 72

FIGURES

Number		Page
1.	Ambient downwind concentrations from test point source under stability A	8
2.	Ambient downwind concentrations from test point source under stability D	8
3.	Downwind ambient concentrations for stability B from point and area sources with transformation	12
4.	Percent secondary sulfate (of sulfur dioxide concentrations) for conditions in Figure 3	12
5.	Downwind centerline concentrations from 1 km square area source for various receptor grid sizes (km) under stability D	13
6.	PEM map of SO_2 concentrations for 1 point and 3 area sources showing receptors where concentrations are calculated	13
7.	PEM map using 2.5 km receptor grid showing concentrations from area sources under stability E and 8 consecutive 45 degree wind shifts	15
8.	PEM map modeling area sources as point sources and stability D, otherwise conditions as in Figure 7	15
9.	Map showing location of point and area sources in the Philadelphia inventory	23
10.	Map showing emission rates of coarse particles from Philadelphia area sources	27
11.	Map showing emission rates of fine particles from area sources	28
12.	Map showing emission rates of SO_2 from area sources	28
13.	Map showing receptor grid of Philadelphia area, sub-census tract areas, city limits and locations of monitors	31
14.	Partial regression plots for 8 source classes	58

TABLES

Number		Page
1.	Comparison of ambient particulate concentrations and fraction of gaseous concentration for test point source for several deposition and settling velocities	9
2.	Summary of TSP, SO_2 and SO_4 emission inventories in the greater Philadelphia area	24
3.	Summary of TSP and SO_2 and SO_4 emission inventories in sources in the local Philadelphia area	25
4.	Primary sulfate emission factors	27
5.	TSP source class contributions from PEM using hypothetical meteorology under three stability categories	32
6.	SO_2 and SO_4 source class contributions from PEM using hypothetical meteorology for three stability categories	33
7.	Average percent TSP source class contributions from PEM using hypothetical meteorology	34
8.	Average percent SO_4 source class contributions from PEM modeling using hypothetical meteorology	34
9.	Meteorological data used in PEM simulation	36
10.	TSP source class contributions using actual meteorology	38
11.	SO_2 and SO_4 source contributions using actual meteorology	39
12.	Apportionment of hourly SO_2 and SO_4 concentrations at selected city receptors for 12 wind directions	41
13.	Differences between classes of receptor and dispersion models	46
14.	Source signatures from Quail Roost II	46
15.	Proportionate variance decomposition of source profiles	50
16.	Simple correlation of source profiles	50
17.	Variance inflation factors of the source profiles	50
18.	Results of all possible regression procedure using synthetic data and Mallow's C_p statistic.	54
19.	Estimated CMB source apportionment using 8 source classes	57
20.	DFBETAS row deletion statistics for CMB of synthetic data set	57

SECTION 1

INTRODUCTION

This is the final report for the April-October 1983 phase of the EPA-MIT Cooperative Agreement examining aerosol models and their applications. The principal objective of this work is to assess the two fundamental approaches to source apportionment of aerosol concentrations: source-oriented dispersion modeling (DM) and receptor modeling (RM). We aim to define the strengths, limitations, areas of applicability and possible protocols for the use of these methods in the regulatory context. The specific objectives include:

(1) Assessment of the new Particle Episodic Model (PEM), a dispersion model which incorporates deposition, settling and transformation processes into the standard Gaussian plume dispersion algorithm. PEM is an extension of the Texas Episodic Model (TEM-8). This report contains a discussion of the verification, applicability and limitations of PEM. Suggestions are given to improve the versatility of the model. A validation study, in which predicted and observed concentrations are compared, is the next logical step in the model evaluation process.

(2) Review and general comments about receptor models. Part of this project has involved a review of the models and literature that make up the current understanding of receptor techniques, as well as our experience with receptor models and similar statistical problems. The current status and capabilities of RM are discussed, with attention to the potential uses of RM in the regulatory process and the application of diagnostic tools to RM which might be part of the modeling protocol.

(3) Discussion of potential hybrid dispersion-receptor models. There are a number of ways to combine source and receptor models. Currently, it is not clear that hybrid models are feasible and desirable. However, it is clear that contributions from each approach can be made to improve the other technique in certain circumstances. Recommendations are made

regarding the development and application of hybrid models in inter-model comparisons, such as the Philadelphia Study (below).

(4) Comparison of DM and RM in the Philadelphia Study. In July and August of 1982 data were collected in the Philadelphia area, in part to compare source apportionments from DM and RM on the same, real data. Ground rules and certain specific tasks are required to make that comparison as meaningful as possible. Guidelines and a discussion of issues for this comparison are presented. Preliminary modeling results using PEM and a source inventory compiled for the Philadelphia area are given.

Data from the Philadelphia Study were not available for this report. Consequently, much of the analysis of receptor models contained herein is theoretical or hypothetical. Further analysis using both real and appropriate synthetic data will be required to determine the value and application of the proposed approaches.

SECTION 2

CONCLUSIONS AND RECOMMENDATIONS

A new dispersion model, the Particle Episodic Model (PEM), was found to successfully incorporate deposition, gravitational settling and linear transformation processes to the predecessor model, the Texas Episodic Model. Thus, PEM should permit greater realism in urban scale modeling. However, some improvements to area source calculations seem warranted.

Application of PEM to a source inventory for the Philadelphia area and a sensitivity analysis indicate:

(1) Area source emissions may dominate TSP, SO_2 and sulfate concentrations at receptors located within an urban scale. Therefore, source inventory data for area sources, including source strengths, operating schedules, micro-inventories (around receptor sites) and the degree and method of aggregation of small sources may be critical to accurate dispersion modeling. Distant sources warrant less attention.

(2) A large fraction of the observed inhalable particle (IP) mass, particularly sulfate, probably comes from medium and long range transport and not from local sources. Preliminary modeling has shown that sulfate contributions from local sources are generally only a few ug/m^3, compared with measured values which average about 24 ug/m^3. However, the modeling examined a relatively short period, and the source inventory is known to be very approximate.

(3) Particle and gaseous concentrations from middle to far field sources (greater than 10 km) may be sensitive to deposition velocities, with greater effects at larger distances. For these sources, gravitational settling is relatively unimportant. Gravitational settling may be important only for sources located in the vicinity of monitors which emit large particles with high settling velocities.

(4) Sulfate concentrations from distant sources are sensitive to transformation rate, especially at low wind speeds.

Our review of the literature and experience with receptor models indicate:

(1) The temporal and spatial variation of source profiles, and the sensitivity of estimated apportionment to such variation is largely unknown. The amount of data needed for representative and useful results is also poorly defined.

(2) Generally, RM studies have been custom designed, including selection of source signatures, filters and analysis. A high degree of subjectivity may be involved in the interpretation and use of data and models.

(3) Each type of RM is prone to certain failures and limitations. Chemical mass balance RMs are subject to problems of collinearity and influential points. Diagnostic procedures can be used to determine whether these problems exist; remedial procedures may be able to minimize their effects. Standardized protocols may be required to ensure meaningful results and promote appropriate uses of RMs.

Both dispersion and receptor models have useful attributes for the source apportionment of aerosols. Dispersion models are predictive and diagnostic. Receptor models are primarily interpretive. Standardized uses of receptor approaches are possible; however, their applicability and limitations need to be defined.

Hybrid models, which combine aspects from both dispersion and receptor approaches, may have application to many air pollution problems, including apportionment of ambient concentrations of criteria and hazardous pollutants, visibility impairement and acid deposition. However, at present, hybrid models are poorly developed and defined. The development and validation of hybrid models will require an extensive data set for various conditions and localities.

SECTION 3

EVALUATION OF THE PARTICLE EPISODIC MODEL

The Particle Episodic Model (PEM) is based on the Texas Episodic Model, Version-8. The new model successfully incorporates simplified deposition, gravitational settling and linear transformation processes into the predecessor model. PEM simultaneously calculates concentration and deposition over an urban scale area in a rectangularly gridded receptor network. A discussion of the the underlying concepts and algorithms in PEM may be found in Rao (1983).

With respect to deposition, PEM provides greater flexibility and some increased realism over comparable models. For example, the ISC model simulates gravitational settling by tilting the (normally horizontal) plume centerline; deposition is modeled by the partial reflection of the source contribution. Settling and deposition processes alter the distribution of mass within the plume. The ISC models's treatment is not altogether statisfactory since it does not model the modified distribution. Consequently, the ISC model tends to overpredict concentrations near the source and underpredict concentrations at large distances. However, as shown later, deposition and gravitational settling only slightly affect concentrations on the urban scale (less than 60 km), especially for the expected range of settling and deposition velocities of inhalable particles.

PEM VERIFICATION

Code Transferral and Compilation

The PEM source code was checked for obvious errors or omissions. No mistakes were found. The source code was then compiled on the IBM FORTRAN VS compiler. Only one "block data" per program is permissible with this compiler. The source code was modified accordingly.

Comparison to TEM-8

PEM was used with simple source and meteorological conditions in each stability category. Results were compared to the TEM-8 model. This showed

good agreement provided that the TEM time step was specified to be 10 minutes. Both models use the same P-G-T dispersion coeffients, but TEM increases these coefficients depending on averaging time. PEM uses these coefficients for calculating one hour averages. (The basic averaging period in PEM is one hour, in TEM, 10 minutes.) Maximum differences between the two models were under a few percent. However, under the most stable categories at relatively long downwind distances, maximum differences could range up to about 30 percent. These differences occur since TEM uses "look-up" tables for dispersion coefficients at discrete distances, while PEM uses piece-wise approximations. While both methods should be sufficiently accurate for model applications, the piece-wise approximations in PEM may provide more consistent results.

Deposition and Settling

An analysis was performed to verify the model's response and sensitivity to changes in settling and deposition velocities. The settling velocity W increases proportionally to the particle density and the square of particle diameter for particles ranging from about 0.05 to 300 um in diameter. Mechanically generated particles, with diameters from about 2 to 50 um, have settling velocities around 1 cm/s. The settling velocities of sulfate and SO_2 are believed to be about 1 to 3 orders of magnitude smaller than the above value (Sehmel, 1980).

The deposition velocity V is the deposition flux divided by the airborne concentration. Deposition velocities are functions of micrometeorological variables (aerodynamic roughness); particle properties (diameter, density, solubility); surface properties (surface roughness and moisture); and measurement height (usually 1-1.5 m). Deposition is difficult to measure and the uncertainties are large. Recommended SO_2 deposition velocity estimates range from 0.04 to 7.5 cm/s (National Academy of Science, 1983); SO_4 deposition velocities are generally less than 1 cm/s. For large particles (greater than 50 um), where gravitational settling is the primary removal mechanism, $V=W>0$. In the case of a gas with perfect reflection from surfaces, $V=W=0$. The effect of both settling and deposition is proportional to V/u and W/u, respectively, where u is the wind speed.

In general, deposition velocities are greater than or equal to the

gravitational settling velocity. PEM does not permit W>V>0, representing, for example, re-entrainment of deposited particles in a dust storm or soil erosion during high winds. Such situations can be modeled as area sources with emission rates which depend on wind speed.

The effect of varying deposition velocity V and settling velocity W (in cm/s) is shown in Figures 1 and 2 and Table 1. These examples use a test point source with a 1 g/s emission rate, 0.13 m diameter stack 10 m high, exit velocity of 35 m/s, and exhaust temperature of 400°K, giving an effective plume release height of 17 m. Meteorological conditions are stability A (Figure 1) and D (Figure 2), and 3 m/s winds. For small distances (< 2 km) and 3 m/s winds, increasing either the deposition or settling velocity from 0 to 10 cm/s results in less than 10 percent change of ambient concentrations with the test point source under stability A (Figure 1) and about 100 percent under stability D (Figure 2). Maximum concentrations occur about 0.5 km downwind under stability category D.

In contrast to near field circumstances (within 1 to 2 km away), concentrations from middle to far field sources (greater than about 10 km distant) may be very sensitive to settling and deposition velocities. Table 1 shows the fraction of the gaseous concentration (i.e., V=W=0) that results with selected deposition and settling velocities using the test point source and the meteorological conditions (Stability D) in Figure 2. For these conditions, concentrations at large downwind distances are sensitive to small deposition velocities (greater than 0.1 cm/s) when the settling velocity is 0. However, ambient concentrations may be small at these downwind distances. For example, a deposition velocity of 1 cm/s results in 74 percent of the gaseous concentration at 3 km, and 33 percent at 60 km. For deposition velocities above 1 cm/s, concentrations are relatively insensitive to settling velocities from 0 to 1 cm/s. Settling velocities above 1 cm/s, (representative of large particles) may have a large effect, producing considerable near field deposition and low ambient concentrations at large distances.

The incorporation of deposition and settling processes into PEM is

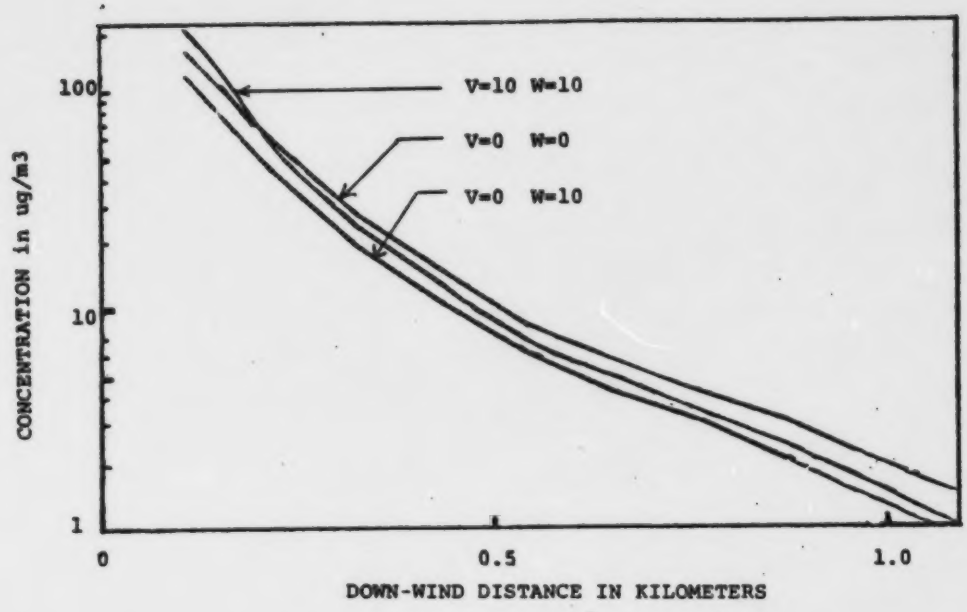

Figure 1. Ambient downwind concentrations from test point source under stability A.

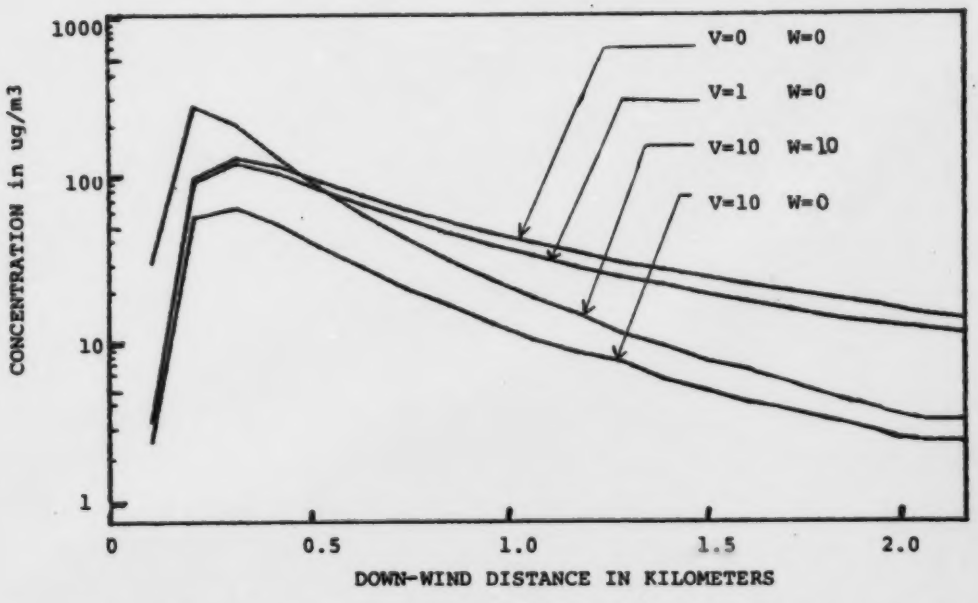

Figure 2. Ambient downwind concentrations from test point source under stability D.

Settling Velocity --cm/s--	Deposition Velocity --cm/s--	--3--	--6--	-15--	-30--	-60--
		Downwind Distance in Kilometers				
		Ambient Concentration of Gas in ug/m^3				
0	0	8.677	2.978	0.799	0.297	0.111
		Ratio of Aerosol Concentration to Gaseous Concentration				
0	0.01	0.997	0.996	0.992	0.990	0.982
0	0.10	0.969	0.957	0.934	0.909	0.874
0	1.00	0.736	0.662	0.534	0.434	0.333
0	10.00	0.139	0.086	0.040	0.024	0.009
0.01	1.00	0.737	0.664	0.537	0.434	0.339
0.10	1.00	0.749	0.667	0.552	0.451	0.342
1.00	1.00	0.877	0.819	0.708	0.606	0.477
2.00	2.00	0.759	0.652	0.474	0.330	0.189
10.00	10.00	0.125	0.038	0.001	0.000	0.000

Table 1. Ambient concentrations and concentration ratios (fraction of gaseous concentration) for test point source and specified deposition and settling velocities.

expected to produce only small changes in gaseous and IP concentrations since local sources are the primary contributors of ambient concentrations (excluding regional contributions). Longer distances are required for significant settling and deposition with the typical range of velocities, but concentrations are low at these distances. This was corroborated using various meteorological scenarios and PEM modeling with the Philadelphia source inventory (Section 4). Varying deposition and/or gravitational velocities from 0 to 1 cm/s changed ambient concentrations by less than 1 percent at most receptors.

Transformation

Figure 3 shows PEM results for primary (SO_2) and secondary (SO_4) pollutants from a point source and an area source of equal strength, using a transformation rate of 1 percent per hour. No primary emissions of SO_4 were assumed. Figure 4 shows that sulfate concentrations, as a fraction of SO2 concentration, increase proportionally with residence time (or downwind distance) for the point source. Sulfate concentrations decline, however, with residence time due to dilution. For the area source, the sulfate fraction increases to a downwind distance of 7 km, whereupon it vanishes due to a cut-off in the PEM program (see below).

For low wind speeds and a typical transformation rate of 1 percent per hour, the transformation of SO_2 emitted within an urban area may constitute a large fraction of ambient SO_4 concentrations. Since primary emissions of SO_4 generally are between 1.5 and 14 percent of primary SO_2 emissions (the Philadelphia inventory averaged 4.3 percent), only several hours residence time is necessary for secondary sulfate to exceed the primary sulfate.

Concentrations from point sources beyond a distance of 60 km are ignored in PEM. This may lower the level of predicted secondary pollutants since there may be insufficient time for significant transformation within 60 km of travel. Concentrations from area sources are calculated for only the four downwind grid cells, which explains the sudden drop at 7 km in Figures 3 and 4. Consequently, the contribution of secondary pollutants from area sources is underestimated.

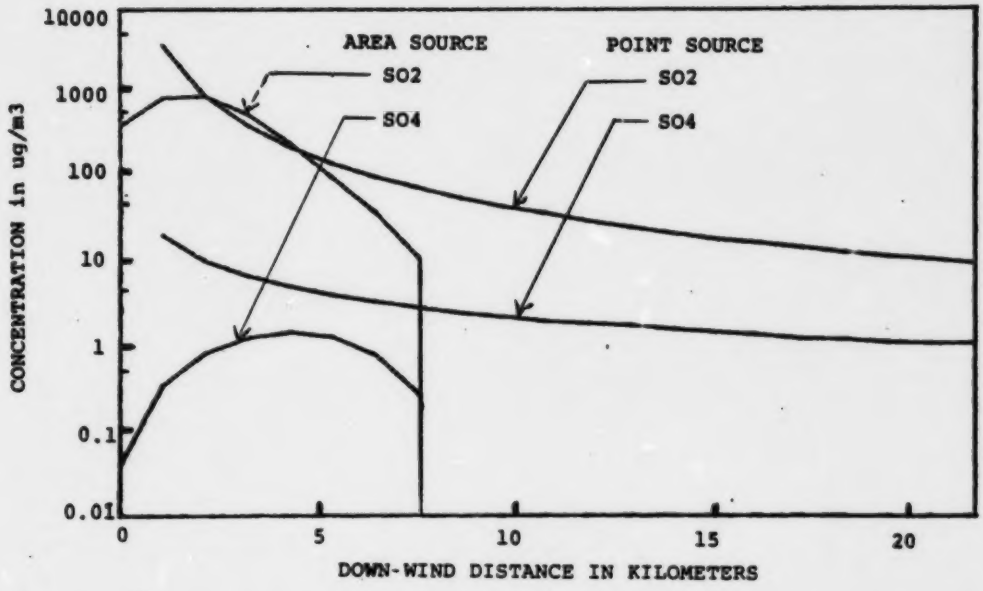

Figure 3. Downwind ambient concentrations for stability B, 0.5 m/s winds. One point source (1 g/s, 0 plume rise); no secondary emissions; one area source (1 g/s, 100 m square); transformation rate of 1 percent/hour.

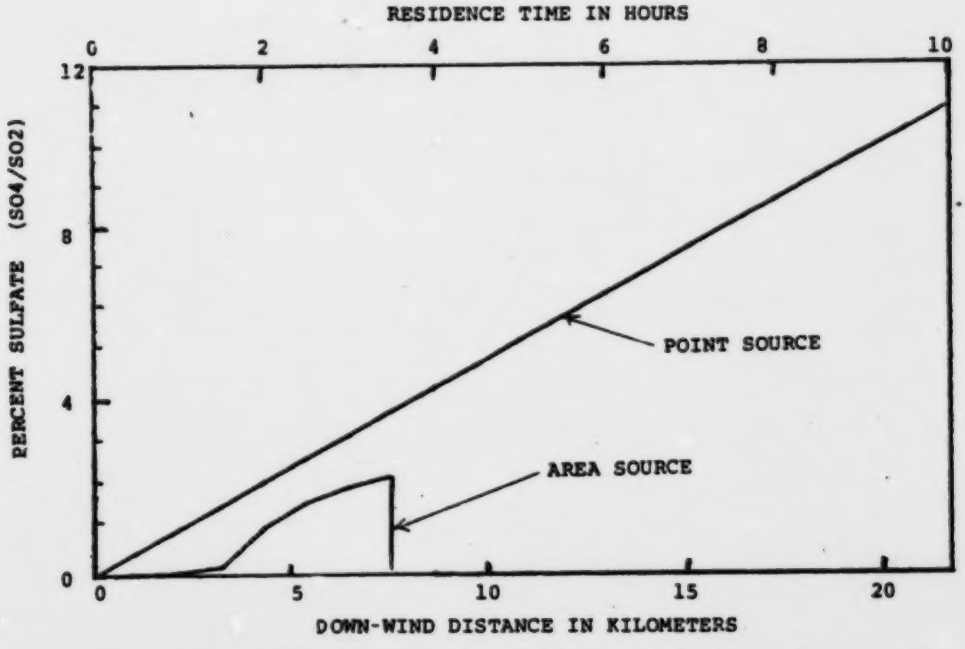

Figure 4. Percent secondary sulfate (of sulfur dioxide concentrations) for conditions in Figure 3.

Area Sources

Area source predictions were compared to "equivalent" ground level point sources. PEM calculates area source contributions in only the four downwind areas in a pattern selected by the program and within the area source itself. If the receptor grid size chosen is very small, a zero concencentation will result not far downwind of the area source. Figures 3, 4, 5 and 6 show that SO_2 and SO_4 concentrations vanish at preselected distances downwind of the area source. This treatment may underestimate the buildup of both primary and secondary pollutants, especially for area sources which are near or smaller than the receptor grid size. Thus, receptor grid size should be choosen so as not to loose important area source contributions.

Area source calculations in PEM automatically decrease the stability category by one, in order to better simulate dispersion under urban condition. All else being equal, concentrations produced by stability category A and B are the same for area sources, while they differ for point sources. This treatment may be anomalous since many urban point sources have low stack heights and undergo similar dispersion conditions as area sources.

Area source modeling is sensitive to the size of the receptor grid. Figure 5 shows downwind centerline concentrations from a 1 km square area source with different receptor grid sizes. The maximum concentration from the area source is produced by a 0.5 km receptor grid. Receptor grid sizes larger than the area source (e.g., 2.5 km grid) result in low concentrations since PEM increases the dimension of (small) area sources to the grid cell size and correspondingly reduces the source intensity (in g/s/area) of the area source. In comparison to the 1 km receptor grid, fine grids (e.g., 0.1 to 0.25 km) produce a somewhat lower maximum concentrations and rapid decrease in ambient concentrations with distance.

The concentration pattern for the four receptors downwind of area sources (selected by the program depending on the wind direction) may not be realistic. Figure 6, a map of ground level concentrations generated by PEM, shows concentrations produced by three area sources (0.1, 1, and 5 km on a side) and a ground level point source without plume rise. All sources have equal source strength. In contrast to the area sources, dispersion from the

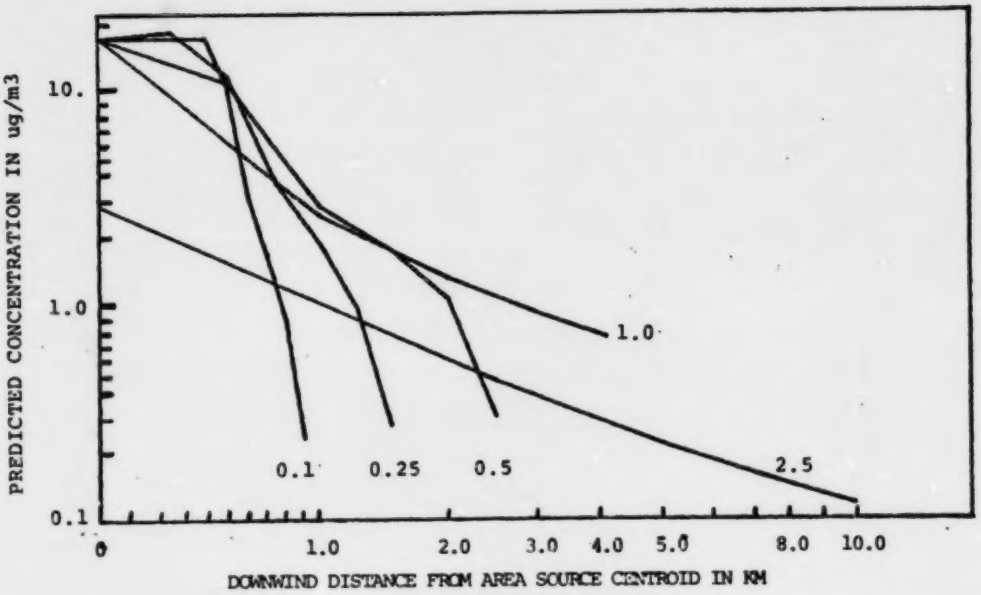

Figure 5. Downwind centerline concentrations from 1 km square area source with specified receptor grid sizes (km); stability D; 3 m/s winds; 1 g/s emission rate;

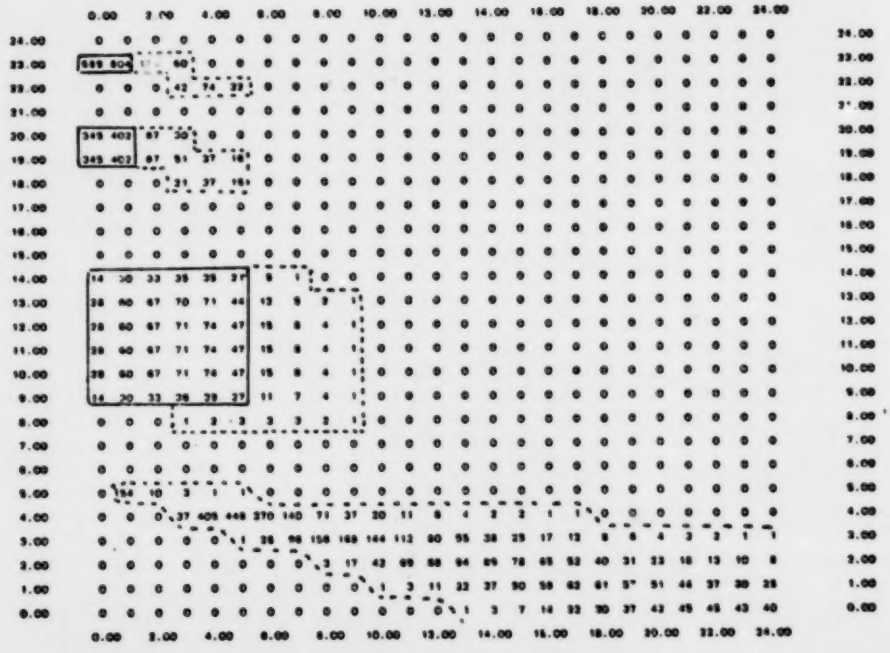

Figure 6. PEM map of SO_2 concentrations from (top to bottom) 3 area and 1 point source; each source has 1 g/s emission rate; solid lines indicate area sources; dashed lines show receptors where concentrations are calculated.

point source affects markedly more downwind receptors. Point source concentrations 20 km downwind are still 20 percent of peak concentrations. Area sources influence a more restricted set of receptors and concentrations decrease more quickly with distance. (The lower stability category used for the area source explains only part of this effect.) Also, the pattern for the four downwind cells leaves large gaps in coverage.

To examine the above effects in urban scale modeling the Philadelphia area sources were described as area sources (2.5 km square in size) in one simulation, and as point sources (with ground level release height and no plume rise) in a second simulation. Both coarse (10 km) and fine (2.5 km) grids were used to obtain eight hour average concentrations under consecutive 45 degree shifts in wind direction and stability D. Stability categories for area sources were increased by one to permit comparison with point sources. In the vicinity of the sources, modeling using area sources produces higher concentrations than point sources (Figure 7 and 8). However, since area source concentrations are calculated only over 4 grid cells downwind, receptors located beyond 10 km (4 x 2.5 km) have zero concentrations using area sources, but non-zero concentrations using point sources. Effects of super-position of point source plumes may result in low (2-3 percent of maximum) concentrations 20 or 30 kilometers downwind (seen, for example, in the NE direction in Figure 7).

There was generally good agreement between area and point source modeling using the coarse grid; concentrations were within 7 ug/m^3 (of an average ambient concentration of 50 ug/m^3) and perimeter concentrations were within 2 ug/m^3 (average of 3 ug/m^3).

In summary, area source modeling is affected by a number of factors. The agreement between point and area source modeling depends critically on the area source dimensions relative to the mean distance between sources. Similarly, the agreement between area source modeling using various grid sizes depends on the area source dimension relative to the receptor grid size. Accurate modeling of near field circumstances may require fine receptor grids, appropriate to the micro-inventory scale. A coarser grid may be used to esimate mid and far field contributions. Total concentrations would be estimated as the sum of the two predictions.

	470.00	475.00	480.00	485.00	490.00	495.00	500.00	505.00	510.00
4450.00	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
4447.50	0	0	0	0	0	0	0	0	0
4445.00	0	0	0	0	0	0	0	0	0
4442.50	0	0	1	1	1	1	1	1	0
4440.00	0	1	1	1	2	3	3	3	0
4437.50	0	1	2	2	4	5	5	6	0
4435.00	1	2	3	7	12	20	25	25	0
4432.50	1	2	4	9	24	47	54	63	0
4430.00	1	2	5	9	44	75	82	84	0
4427.50	1	2	6	25	64	75	81	74	0
4425.00	1	3	13	36	71	98	99	86	0
4422.50	1	3	14	27	55	99	114	85	0
4420.00	1	3	5	18	38	62	82	49	0
4417.50	1	2	4	20	31	42	61	39	0
4415.00	1	2	3	14	16	14	30	24	0
4412.50	0	1	2	3	3	4	4	4	0
4410.00	0	1	1	1	1	1	2	1	0
	470.00	475.00	480.00	485.00	490.00	495.00	500.00	505.00	510.00

Figure 7. PEM map using 2.5 km receptor grid showing concentrations from area sources; stability E; and 8 consecutive 45 degree wind shifts.

	471.20	476.20	481.20	486.20	491.20	496.20	501.20	506.20	511.20
4451.20	1 1 1	1 2 2	2 1 1	1 1 1	0 0 0	1 1 1	1 2 2		
4448.70	1 1 1	1 2 2	2 1 1	1 1 1	1 0 1	1 1 1	2 2		
4446.20	1 1 1	2 2 2	2 1 1	1 1 1	1 1 1	1 2 2	2		
4443.70	1 1 1	2 2 3	2 1 1	1 1 1	1 2 2	3 3 2			
4441.20	1 2 2	2 2 3	3 1 1	1 1 1	2 2 3	3 2 1			
4438.70	2 1 2	3 2 3	3 3 1	1 2 3	3 3 3	1 0			
4436.20	2 2 2	4 4 3	5 4 4	3 4 4	4 4 3	1 0 0			
4433.70	3 3 4	6 11 14	9 10 16	16 8 6	5 2 1	0 0			
4431.20	4 4 5	10 20 26	28 25 25	26 28 17	2 1 1	1 1			
4428.70	3 5 5	14 24 31	43 39 32	36 36 12	1 1 1	1 1			
4426.20	2 4 11	20 26 38	40 61 58	30 14 3	3 1 1	1 1			
4423.70	2 4 17	29 55 72	76 65 37	15 3 4	3 3 2	2 2			
4421.20	4 4 13	33 69 102	74 27 10	6 5 2	3 3 2	2 2			
4418.70	2 6 11	21 54 64	48 31 5	3 4 3	2 2 2	2 1			
4416.20	2 4 15	16 22 54	65 21 4	3 2 3	2 2 2	1 1			
4413.70	3 4 7	40 49 39	31 5 7	3 3 2	3 2 1	1 1			
4411.20	3 4 4	40 41 3	2 8 4	5 3 2	2 2 2	3 1 1			
	471.20	476.20	481.20	486.20	491.20	496.20	501.20	506.20	511.20

Figure 8. PEM map modeling area sources as point sources, stability D, otherwise conditions as in Figure 7.

PEM IMPROVEMENTS

We found the PEM model easy to use (even without a users guide). However, the versatility and convenience of the PEM program could be improved. Some of the recommendations in this section result from our experience with the model; others are proposed in view of expected applications. Implementation of the minor changes to the model, e.g., book-keeping operations, additional outputs and new user options, would facilitate a sensitivity analysis and source apportionments. Other changes might increase the realism of the model. The somewhat increased complexity, memory storage and computer time required by the model would not be important considerations to most model users. Incorporating changes before the model is released would be advantageous since user modifications would not be necessary thus eliminating further review by regulatory authorities.

A brief assessment is given below of the importance, objective, and ease of implementing the various possible changes. Many of the suggestions could be included as options (defaults would use the existing program).

Deposition, Settling and Transformation

The current model requires that deposition, settling and transformation parameters pertain to all sources and meteorological conditions in an averaging period (1 to 24 hours). The following suggestions provide a hierarchy of increasing sophistication in handling these processes.

a. Hourly variations of deposition and transformation parameters.

   Importance: Variable, depending on importance of deposition and transformation.

   Objective: Portray time varying characteristics, e.g., day/night differences of deposition velocities.

   Implementation: Programming simple. Little guidance for user. Possibly tied to stability and wind speed inputs.

b. Source-specific deposition, settling and transformation parameters.

Importance: Moderate for calculations of TSP where emission characteristics vary widely. Less important for gases and IP with similar characteristics.

Objective: Increased realism by reflecting different particle size distributions from various sources.

Implementation: Programming simple, but specification possibly difficult (especially if parameters vary on hourly basis) due to incomplete data.

c. Particle size stratification of deposition and settling parameters.

Importance: Generally minor, since size (weighted) average parameters may be used in most cases.

Objective: More accurate description of particle dispersion by reflecting distribution of particle sizes. Also permits simultaneous calculation of TSP, IP, and gaseous pollutants.

Implementation: Programming simple. Handle as additional pollutant (e.g., increase number of pollutants to five and sum pollutants.)

d. Site-specific deposition velocities.

Importance: Moderate, depending if deposition is important.

Objective: Increased realism by modeling surfaces found over large areas, e.g., water, urban, grass.

Implementation: Programming possibly difficult since present solution algorithm may not be suitable. More complicated if deposition changes with time. User must specify surfaces and deposition rates (possibly keyed to surface type.

e. Insignificant transformation rates.

Importance: Minor, depending on transformation rate, source-receptor distances and wind speed.

Objective: Reduced CPU time by eliminating calculations from (numerous) small local sources and meteorology which produces neglible transformation.

Implementation: Moderate programming difficulty. Requires look-up charts and relative estimates of extent of transformation. Invisible to user.

Source Specifications

a. Hourly variations of source strength and other source characteristics (exit velocity, temperature).

Importance: Small for modeling worst case conditions, possibly large for validation and other studies, especially with significant daily variations of emission sources.

Objective: Simulate operating schedules of major emitters.

Implementation: Programming simple. Possibly large amounts of input data.

b. Determination of source class impacts.

Importance: Variable, depending on application.

Objective: Expands culpability option, particularly useful in SIP revision. Also defines culpability of industrial source complex with multiple emission sources.

Implementation: Programming straightfoward, involving additional specification of source classes and book-keeping of class impacts for receptors. User simply specifies source class.

Area Sources

a. Make area source calculations independent of receptor grid size.

Importance: Variable, depending on importance of area sources and receptor grid size chosen.

Objective: Increased realism of area source modeling.

Implementation: Programming possibly difficult. Invisible to user.

b. Concentration and/or other criteria for determination of number of downwind grid cells.

Importance: Variable, depends on importance and configuration of area sources.

Objective: Increased realism of area source modeling by using meaningful standard rather than fixed (4 downwind receptors) calculations.

Implementation: Programming straightforward. Invisible to user.

Outputs

a. Automatic scaling of concentration and deposition flux maps.

Importance: Minor, for convenience.

Objective: Eliminate useless outputs and model runs producing numbers either too small or too large for display.

Implementation: Programming simple. Invisible to user.

b. Culpability list of all (or specified number) of sources at specified receptors showing major contributors to receptor concentrations.

Importance: Normally minor, since culpability of top 10 point sources is provided. However, expand to include area source contributions.

Objective: Facilitates source apportionment, especially in validation.

Implementation: Programming and use straightforward.

c. Hourly concentrations written on tape.

Importance: Minor, but convenient. Present option writes only final (1 to 24 hour) average concentrations on tape.

Objective: Permits analysis of critical meteorological conditions, etc.

Implementation: Trivial.

Miscellaneous

a. Hourly variations of calibration parameters, particularly intercept.

Importance: Minor.

Objective: Portray changes of background levels.

Implementation: Simple.

b. User specification of wind profile exponents and anemometer height.

Importance: Generally minor.

Objective: Tailor model to location, if estimates are available.

Implementation: Simple.

c. Incorporate varying terrain.

Importance: Potentially large with elevated sources and complicated terrain.

Objective: Model fumigation of elevated terrain.

Implementation: Programming difficult, since algorithms may not be suitable and deposition and settling processes poorly understood with terrain differences. Usage simple by specifying receptor elevation.

d. Increase or eliminate cut-off distance for point sources

Importance: Possibly important with certain emission inventories.

Objective: Extends modeling to mesoscale (30-300 km).

Implementation: Trivial.

e. Use of updated dispersion coeffiecients

Importance: Important under some conditions

Objective: Standardize models with other UNAMAP models

Implementation: Trivial

e. Long Term Version of PEM

A long term version of PEM could be very useful. Such a model might be similar to the ISC-LT model, which calculates annual concentrations using site-specific meteorological data. The joint probability of the STAR categories, i.e., each wind speed, wind direction and stability category, is used to weight ambient concentrations for that category in the determination of annual or seasonal average concentrations. This would yield spatially varying long-term concentrations that might be more valid than short-term concentrations predictions, which depend on accurate source and meteorological data.

SUMMARY

Of the recommended changes, we feel that the most important improvements increasing model credibility are those concerning area source modeling. For sulfate modeling, hourly variation of transformation rates and elimination of cut-off distances for point and area source calculations are the most relevant. For TSP modeling, source specific specification of particle size or deposition and settling velocity are important. We also feel that the development of a long term version of PEM for seasonal or annual particulate concentrations would complement existing air quality models. Most of the remaining recommendations simply provide greater convenience for model users.

SECTION 4

SOURCE APPORTIONMENT USING PEM

In this section we describe aerosol source apportionment in Philadelphia using the PEM dispersion model. The source inventory, meteorology and PEM predictions are presented. The results could be indicative of the composition of aerosols obtained by dichotomous samplers in the Philadelphia study.

SOURCE INVENTORY

The preliminary source inventory was compiled to obtain the approximate composition and location of the major emission sources in the Philadelphia metropolitan area. Sources of the data are listed at the end of this section. The data do not include micro-inventories around receptor sites. Present data do not allow a complete classification of sources. However, this should not seriously handicap the apportionment since the objective is to obtain only representative inventory and source apportionment estimates. More detailed source and monitor data for the Philadelphia study should permit more accurate modeling.

The inventory consists of a total of 50 area sources and 104 point sources. The location of the sources is shown in Figure 9. Particle emissions are broken down into 12 source classes as shown in Table 2. This Table also shows the six source classes of SO_2 and (primary) SO_4 sources.

The composition of the emissions sources located within the city is different than shown in Table 2, which includes a number of large sources located up to 60 km from the city limits. Table 3 provides a summary of the emission sources located within 470 to 500 UTM east, and 4410 to 4440 UTM north, a region which encompasses Philadelphia city limits with the exception of the northeast corner (see Figure 13). In this smaller region, area sources emit most of the TSP and a few industrial sources emit most of the SO_2 and SO_4.

Area source emissions included both fine and coarse particles, as well as SO_2 and SO_4. Area source emissions were estimated by aggregating about 600 sub-census tract emission estimates into fifty 2.5 km square

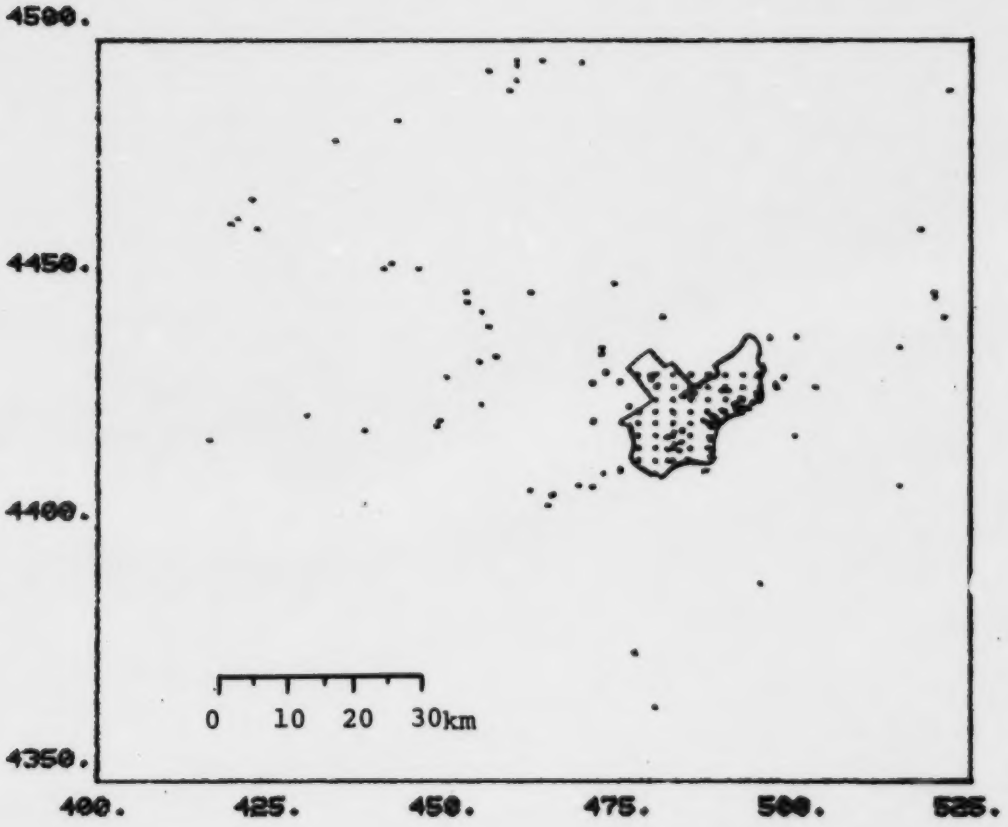

Figure 9. Map showing location of 104 point sources and 50 area sources used in the Philadelphia inventory. Philadelphia city limits are shown in the center of the figure. Scales are UTM coordinates.

	Category	Number of Sources	---TSP Emissions-- g/s	percent
1	Area sources--coarse	50	246.18	14.1
2	Area source--fine	50	17.23	9.9
3	Refineries	7	127.30	7.3
4	Incinerators	5	39.54	2.3
5	Oil-fired utility	8	299.39	17.2
6	Coal-fired boilers	14	287.10	16.5
7	Metal and steel	9	280.33	16.1
8	NJ County Emissions	6	266.00	15.3
9	Chemical industries	10	77.89	4.5
10	Grain elevator	1	25.92	1.5
11	Misc. ground level	3	24.65	1.4
12	Misc. oil-fired	40	50.76	2.9
	Totals	203	1742.26	100

	Category	Number of Sources	SO_2 Emissions g/s	percent	SO_4 Emissions g/s	percent
1	Area sources	56	317.48	5.0	22.14	8.0
2	Oil--industrial	8	1531.25	23.8	107.19	38.6
3	Coal	14	2335.00	36.4	35.04	12.6
4	Oil--miscellaneous	40	525.18	8.2	27.22	9.8
5	Chemical industries	9	245.10	3.8	13.89	5.0
6	Refineries	7	1457.30	22.7	72.57	26.1
	Totals	134	6411.31	100	278.05	100

Table 2. Summary of TSP (top) and SO_2 and SO_4 (bottom) emission inventories in the Philadelphia area.

	Category	Number of Sources	---TSP Emissions-- g/s	percent
1	Area sources--coarse	50	246.18	37.8
2	Area source--fine	50	17.23	2.6
3	Refineries	4	95.70	14.7
4	Incinerators	5	39.54	6.1
5	Oil-fired utility	6	60.19	9.2
6	Coal-fired boilers	2	66.30	10.2
7	Metal and steel	4	25.11	3.9
8	NJ County Emissions	0	0.00	0.0
9	Chemical industries	6	19.29	3.0
10	Grain elevator	1	25.92	4.0
11	Misc. ground level	3	19.15	2.9
12	Misc. oil-fired	22	36.59	5.6
	Totals	153	651.20	100

	Category	Number of Sources	SO_2 Emissions g/s	percent	SO_4 Emissions g/s	percent
1	Area sources	50	249.15	12.0	17.23	10.5
2	Oil--industrial	6	1222.96	58.7	85.61	52.3
3	Coal	2	502.10	24.1	7.53	4.6
4	Oil--miscellaneous	22	436.98	21.0	13.10	8.0
5	Chemical industries	6	223.70	10.7	12.80	6.5
6	Refineries	4	548.00	26.3	27.47	16.7
	Totals	90	2083.19	100	163.68	100

Table 3. Summary of TSP (top) and SO_2 and SO_4 (bottom) emission inventories in Philadelphia located within 470 to 500 UTM east and 4410 to 4440 UTM north.

areas. The area source inventory combined emissions from mobile, point and area source emissions. However, coarse TSP emissions are primarily from road dust; fine TSP emissions are from mobile sources and residential and commercial activities; and SO_2 emissions are primarily from residential oil-fired burners. Figures 10 to 12 show area source estimates for the three pollutants.

Primary SO_4 emissions were determined by multiplying SO_2 emissions by the factors given in Table 4 (National Research Council, 1983). Thus, all SO_2 sources had primary sulfate emissions. Area sources had a emission weighted sulfate emission factor of 7 percent. The emission weighted sulfate emission factor for the entire inventory is 4.3 percent.

The inventory was compiled from the inventories listed below:

1. City of Philadelphia Air Management Services, Philadelphia, PA. B. Glazer, T. Weir, (215) NU6-7893

   Comprehensive inventory of city emission sources listing over 1000 point sources including hazardous pollutant emissions and area source emissions of fine and coarse particulates, SO_2, SO_4, NOx. Limited computer capability.

2. PEDCO Micro Inventory, PEDCO Environmental, Cincinnati, OH. Barb Siegal, (513) 782-4700

   Major TSP point sources (over 100 T/yr) in the Philadelphia area. Completed for 1978 monitoring study. 1982-3 update forthcoming.

3. N.J. State Dept. of Environmental Protection, Bureau of Field Operations. Trenton office: Dr. Ray Dyba, (609) 985-3009; Cherry Hill, Camden County office: Terry Juchnowski (609) 984-0616

   Estimates of criteria pollutant emissions and identification of major sources for Burlington, Camden, Glousester and Mercer Counties. Not computerized (on microfiche).

4. Pennsylvania Department of Environmental Resources, Inventory section, Harrrisburg, PA. John Walker (717) 787-4324

   PA point sources (excluding those located in the City of Philadelphia) including emissions of criteria and other pollutants, operating schedules and plant parameters. Sophisticated computerized inventory.

-------Fuel----------	--Percentage Primary SO_4--
Coal	1.5
Residual oil--industrial	7.0
--residential	13.4
Distillate oil	3.0
Mobile sources	3.0
Miscellaneous	5.0

Table 4. Primary sulfate emission factors (National Research Council, 1983).

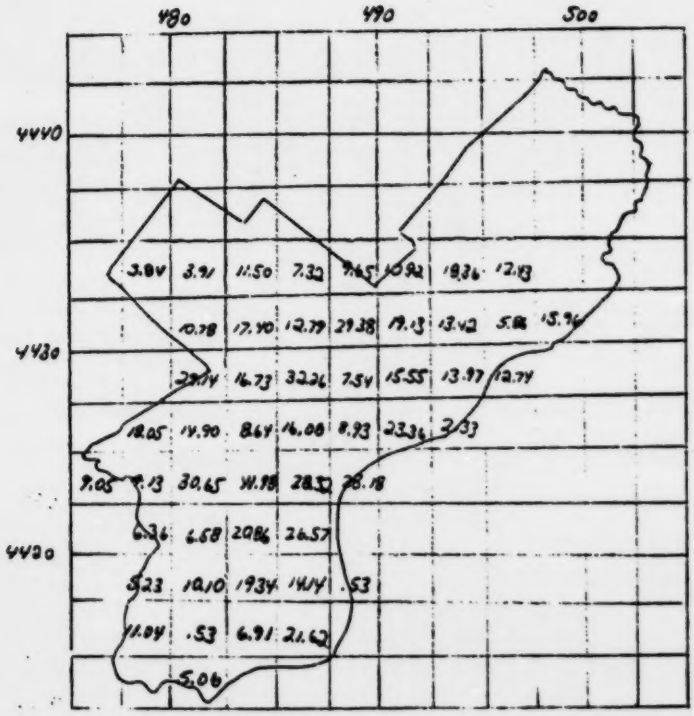

Figure 10. Map showing emission rates (g/s) of coarse particles from Philadelphia area sources. Area sources are 2.5 km square.

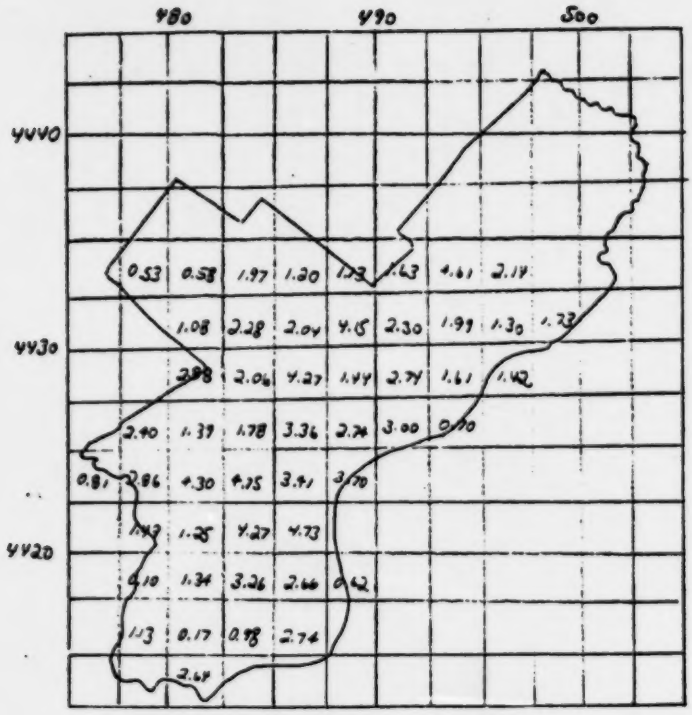

Figure 11. Emission rates (g/s) of fine particles from area sources.

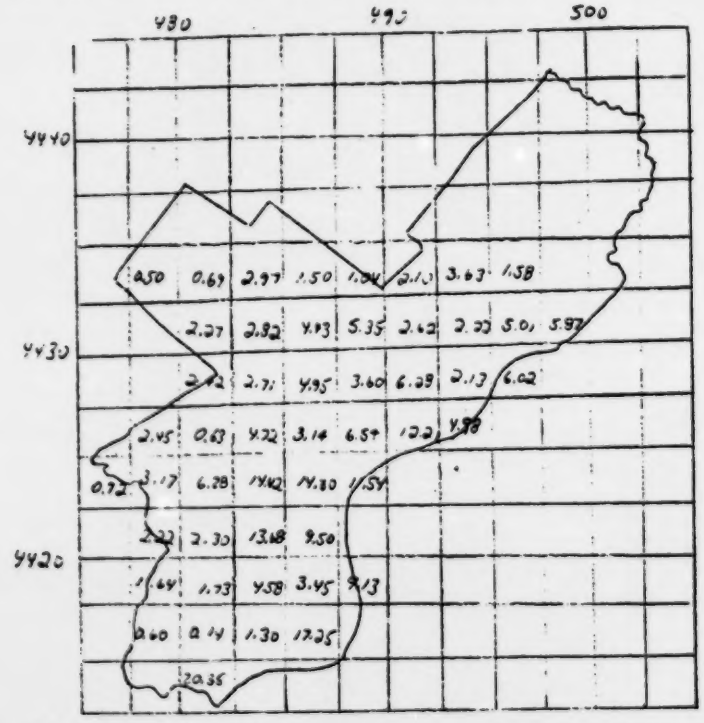

Figure 12. Emission rates (g/s) of SO_2 from Philadelphia area sources.

5. "Thermal Electric Power Plant Contruction and Annual Production Expenses," Energy Information Administration, Washington, D.C., 1980.

Several power plant emissions were estimated using these fuel records and maximum NSPS emissions.

METEOROLOGY

Surface meteorological data for the PEM simulation were obtained for the Philadelphia's Northeast airport and the Norristown meteorological station. The Norristown data were received in a preprocessed format, which included stability classifications. No mixing heights were obtained. PEM simulations used constant, ficticious mixing heights (as specified).

These data were obtained from:

Pennsylvania Department of Environmental Resources, Meteorology Section, Harrisburg, PA. Denis Lohman (717) 787-4319

DISPERSION MODELING

The PEM dispersion model was used to estimate the source apportionment in the Philadelphia area under several meteorological scenarios. PEM can simulate dispersion of either two independent pollutants, or one pair of coupled pollutants. Thus, source apportionment of the 12 TSP source classes was accomplished by 6 model runs, each run modeling two (independent) source classes. Source apportionment of SO_2 and SO_4 for the 6 source classes required 6 model runs, since SO_2 to SO_4 transformation was permitted and each source emitted both SO_2 and primary sulfate. A constant 1 percent per hour transformation rate was used. Deposition and gravitational velocities were set to zero. A tape output of concentrations at each receptor was generated by each model run. After the 6 runs for each apportionment (and meterological scenario) were completed, a Conversational Monitoring System (CMS) "macro" program consolidated the concentrations into one file, which was then transferred to the Time-shared Reactive On-Line Laboratory (TROLL), a large, interactive statistical and data analysis system (Information Processing Center, 1980). TROLL was used to generate the source apportionment tables. Both CMS and TROLL reside on the MIT IBM/370 Computer.

Hypothetical Meteorology

First, hypothetical meteorology was used to portray the average effect of the sources at each receptor. Eight hour concentrations were calculated using consecutive hourly 45 degree wind shifts (starting at 0 degrees) using a fine (25 x 25 grid; 60.0 km square) receptor network for the following stability categories and wind speeds:

stability category	wind speed (m/s)
A	2
D	4
E	3

Due to hourly shifts in the wind direction in these scenarios, no single source contributed longer than one hour to receptor concentrations (with the exception of receptors located within area sources).

Based on the results obtained, a coarse (4 x 4 grid; 30 km square, SW corner UTM 4410 north, 470 east) was selected to include both areas of maximum concentration and the Philadelphia monitoring sites. The receptor grid and receptor numbers are shown in Figure 13. This receptor network encompasses Philadelphia and adjoining suburbs. The coarse grid was chosen primarily to reduce computations; it may not reflect the diversity of concentrations at the various monitors in the Philadelphia area.

Predicted source class estimates are given in Table 5 for TSP (excluding sulfate) and Table 6 for SO_2 and SO_4. The average percent source class contributions of TSP and SO_4 at the 16 receptors are listed in Tables 7 and 8. The following results are highlighted:

(1) Receptors show a diverse source apportionment. Receptors 6, 7, 10 and 11, located within Philadelphia, receive high loadings from area sources.

(2) Point sources contribute less than 1 ug/m^3 under stability A compared to up to 60 ug/m^3 from area sources. Point sources have larger contributions under other stabilities. However, area sources dominate both TSP and SO_2 concentrations.

(3) Low sulfate concentrations, generally about 5 percent of TSP, reflecting the relatively high wind speeds which advect the pollutants outside the area resulting in little SO_2 to SO_4 transformation, as well as the small proportion of primary sulfate.

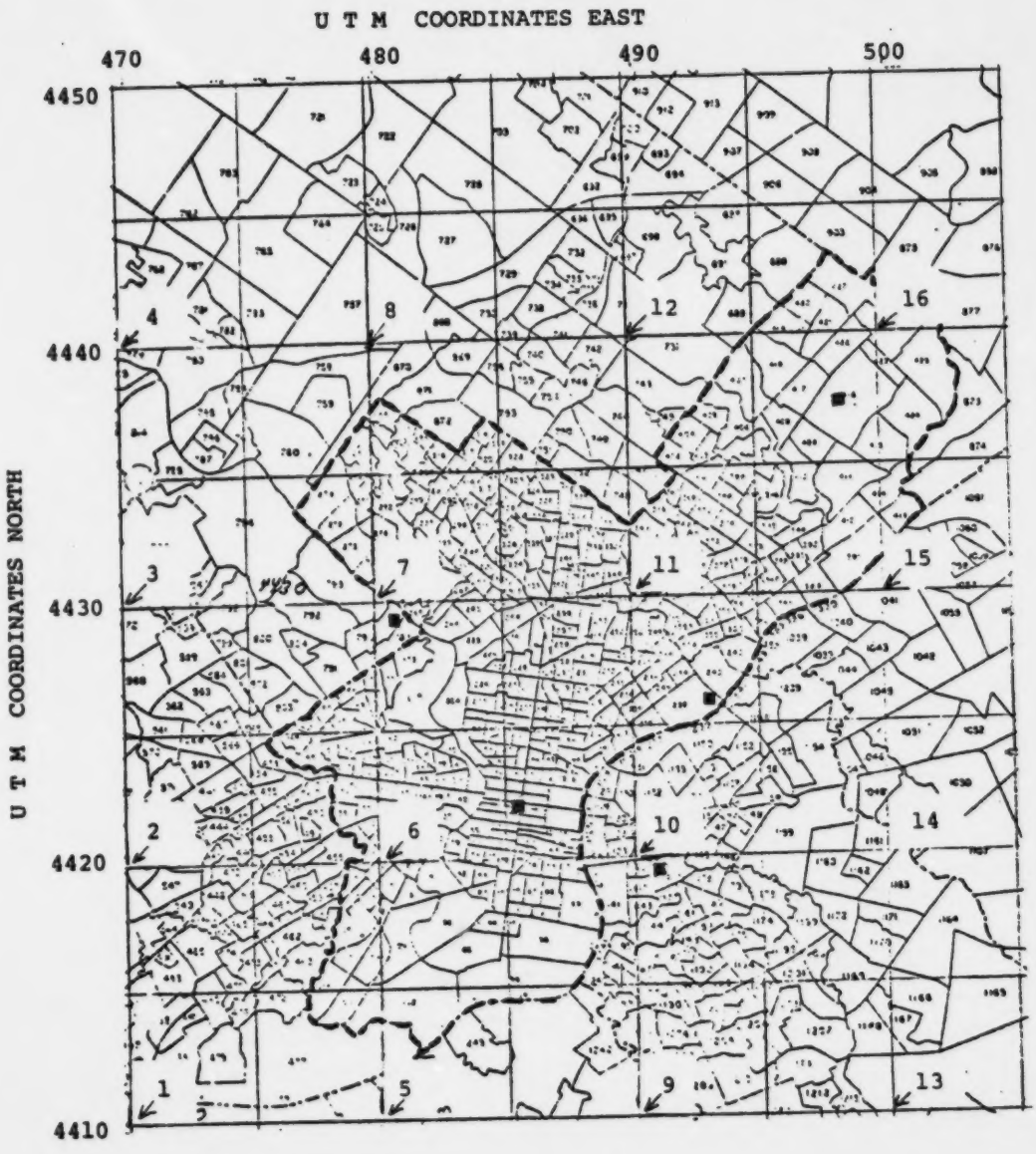

Figure 13. Map showing 5 km receptor grid of Philadelphia area. City limits shown with dashed line. Small numbered regions are sub-census tract areas. Large numbers indicate receptor number for coarse (10 km) grid used in modeling. Squares indicate location of five monitors of the Philadelphia study; the sixth is located 7 km south of map.

RECEPTOR NUMBER	SOURCE CLASS CONTRIBUTION IN UG/M3												TOTAL
	AREA-C	AREA-F	REFIN.	INCIN.	OIL-IND	COAL	STEEL	NU-MIS	CHEM.	GRAIN	SOIL	OIL-MIS	CONCENT
1.....	1.807	0.288	0.037	0.018	0.541	0.513	0.013	0.047	0.011	0.003	0.005	0.142	3.427
2.....	1.150	0.164	0.020	0.018	0.095	0.093	0.036	0.057	0.017	0.011	0.002	0.012	1.676
3.....	1.544	0.226	0.073	0.022	0.278	0.066	0.026	0.018	0.034	0.025	0.008	0.028	2.347
4.....	1.054	0.147	0.013	0.016	0.058	0.060	0.187	0.017	0.028	0.003	0.003	0.014	1.602
5.....	1.370	0.200	0.051	0.015	0.110	0.094	0.006	0.077	0.018	0.005	0.012	0.033	1.992
6.....	43.342	5.692	0.158	0.019	0.146	0.081	0.023	0.077	0.059	0.096	0.002	0.039	50.734
7.....	34.380	4.370	0.055	0.057	0.080	0.032	0.043	0.035	0.025	0.007	0.008	0.038	39.087
8.....	1.453	0.218	0.041	0.026	0.082	0.019	0.028	0.049	0.012	0.011	0.014	0.015	1.967
9.....	1.294	0.201	0.169	0.020	0.123	0.059	0.006	0.096	0.012	0.042	0.010	0.031	2.062
10....	30.793	4.598	0.036	0.037	0.125	0.020	0.019	0.104	0.031	0.005	0.011	0.070	35.848
11....	59.744	9.625	0.042	0.349	0.083	0.035	0.006	0.109	0.008	0.003	0.027	0.095	70.096
12....	1.511	0.223	0.023	0.030	0.083	0.021	0.016	0.058	0.013	0.002	0.010	0.021	1.992
13....	1.158	0.156	0.029	0.009	0.093	0.031	0.010	0.122	0.009	0.001	0.002	0.013	1.630
14....	1.551	0.241	0.026	0.030	0.018	0.009	0.005	0.040	0.014	0.013	0.019	0.017	1.984
15....	12.701	1.798	0.071	0.026	0.029	0.019	0.002	0.124	0.008	0.015	0.007	0.048	14.848
16....	1.815	0.284	0.034	0.014	0.083	0.030	0.012	0.082	0.020	0.008	0.002	0.012	2.396
MEAN....	12.290	1.839	0.055	0.044	0.122	0.074	0.027	0.069	0.020	0.019	0.009	0.039	14.606

RECEPTOR NUMBER	SOURCE CLASS CONTRIBUTION IN UG/M3												TOTAL
	AREA-C	AREA-F	REFIN.	INCIN.	OIL-IND	COAL	STEEL	NU-MIS	CHEM.	GRAIN	SOIL	OIL-MIS	CONCENT
1.....	0.924	0.145	0.001	0.101	0.015	0.017	0.018	0.689	0.027	0.000	0.001	0.063	2.002
2.....	1.111	0.159	0.000	0.002	0.015	0.545	0.016	1.220	0.035	0.001	0.000	0.057	3.161
3.....	1.353	0.199	0.246	0.082	1.729	0.271	0.022	0.006	0.337	1.338	0.018	0.220	5.823
4.....	0.611	0.081	0.000	0.042	0.198	0.118	0.943	0.001	0.089	0.000	0.001	0.129	2.211
5.....	1.163	0.171	0.001	0.081	0.031	0.257	0.015	1.416	0.024	0.000	0.076	0.146	3.361
6.....	26.643	4.111	0.154	0.072	1.399	0.309	0.046	2.430	0.260	4.827	0.000	0.200	40.451
7.....	21.297	2.726	0.001	0.032	0.114	0.011	0.003	0.319	0.012	0.000	0.000	0.052	24.567
8.....	1.409	0.211	0.005	0.162	0.019	0.001	0.033	1.291	0.067	0.012	0.402	0.116	3.728
9.....	1.257	0.195	0.004	0.101	1.112	0.164	0.053	4.505	0.063	2.923	0.090	0.089	10.557
10....	19.195	2.868	0.000	0.081	0.007	0.072	0.035	5.590	0.060	0.000	0.000	0.093	27.979
11....	36.484	5.868	0.025	0.000	0.094	0.037	0.024	3.554	0.006	0.000	0.190	0.110	46.392
12....	1.458	0.215	0.018	0.095	0.034	0.004	0.049	0.220	0.042	0.000	0.092	0.209	2.436
13....	0.660	0.093	0.005	0.030	0.272	0.032	0.024	7.905	0.076	0.000	0.000	0.119	9.216
14....	1.503	0.234	0.000	0.105	0.027	0.009	0.009	0.007	0.065	0.006	0.522	0.128	2.614
15....	8.128	1.155	0.009	0.026	0.074	0.019	0.002	5.879	0.018	0.055	0.033	0.355	15.783
16....	1.163	0.163	0.028	0.054	0.136	0.064	0.015	2.172	0.027	0.004	0.000	0.066	3.912
MEAN....	7.772	1.163	0.031	0.064	0.330	0.121	0.082	3.325	0.076	0.573	0.089	0.134	12.760

RECEPTOR NUMBER	SOURCE CLASS CONTRIBUTION IN UG/M3												TOTAL
	AREA-C	AREA-F	REFIN.	INCIN.	OIL-IND	COAL	STEEL	NU-MIS	CHEM.	GRAIN	SOIL	OIL-MIS	CONCENT
1.....	7.889	1.244	0.000	0.181	0.004	0.033	0.035	2.102	0.024	0.000	0.000	0.149	11.661
2.....	9.068	1.294	0.000	0.001	0.007	1.212	0.019	3.688	0.080	0.000	0.000	0.053	15.422
3.....	11.214	1.658	0.751	0.146	4.056	0.468	0.018	0.001	0.988	4.098	0.008	0.593	23.995
4.....	5.170	0.691	0.000	0.064	0.513	0.734	2.652	0.000	0.170	0.000	0.000	0.215	10.208
5.....	9.561	1.400	0.006	0.108	0.044	0.766	0.020	4.251	0.019	0.000	0.049	0.280	16.504
6.....	119.350	18.389	0.478	0.108	3.538	0.746	0.080	7.194	0.768	6.867	0.000	0.422	157.940
7.....	97.089	12.600	0.026	0.029	0.199	0.014	0.011	0.480	0.011	0.000	0.000	0.099	110.557
8.....	11.592	1.743	0.052	0.318	0.042	0.001	0.039	4.017	0.117	0.001	0.966	0.250	19.137
9.....	10.401	1.615	0.069	0.212	3.034	0.493	0.107	14.384	0.115	7.645	0.064	0.310	38.450
10....	88.574	13.223	0.000	0.100	0.009	0.171	0.103	17.280	0.127	0.000	0.000	0.238	119.821
11....	160.990	25.805	0.104	0.000	0.201	0.159	0.011	10.403	0.004	0.000	0.052	0.192	197.921
12....	11.860	1.747	0.007	0.152	0.032	0.035	0.088	0.133	0.047	0.000	0.081	0.318	14.479
13....	5.625	0.788	0.082	0.074	0.656	0.210	0.129	24.851	0.157	0.000	0.000	0.203	32.775
14....	12.334	1.919	0.002	0.189	0.014	0.038	0.002	0.000	0.116	0.000	0.749	0.214	15.576
15....	39.646	5.682	0.011	0.021	0.118	0.025	0.002	17.238	0.021	0.017	0.046	0.717	63.544
16....	9.741	1.533	0.148	0.073	0.257	0.232	0.031	6.330	0.041	0.000	0.000	0.169	18.553
MEAN....	38.131	5.708	0.108	0.111	0.795	0.334	0.209	7.022	0.175	1.164	0.125	0.278	84.158

Table 5. TSP source class contributions from PEM using hypothetical meteorology (8 consecutive 45 degree shifts in wind direction). Top: stability A; Middle: stability D; Bottom: stability E.

RECEPTOR NUMBER	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
1.....	0.000	5.558	5.212	1.409	0.110	0.856	13.146	0.000	0.412	0.090	0.104	0.011	0.065	0.671
2.....	0.000	0.855	0.592	0.138	0.109	0.150	1.842	0.000	0.079	0.024	0.010	0.009	0.011	0.133
3.....	1.558	1.817	0.491	0.382	0.127	0.528	4.883	0.238	0.158	0.028	0.032	0.011	0.047	0.514
4.....	0.848	0.503	0.440	0.155	0.214	0.252	2.410	0.101	0.058	0.038	0.014	0.015	0.028	0.255
5.....	0.178	0.857	0.956	0.364	0.086	0.616	3.038	0.017	0.078	0.047	0.029	0.006	0.045	0.222
6.....	12.229	0.731	0.678	0.442	0.510	1.354	15.943	0.941	0.072	0.041	0.034	0.029	0.097	1.214
7.....	6.280	0.533	0.033	0.458	0.187	0.448	7.939	0.476	0.048	0.002	0.021	0.014	0.039	0.599
8.....	1.685	0.565	0.151	0.170	0.057	0.244	2.871	0.180	0.053	0.013	0.014	0.005	0.023	0.289
9.....	0.479	0.689	0.539	0.353	0.051	1.201	3.312	0.049	0.079	0.035	0.028	0.005	0.090	0.285
10....	12.015	1.168	0.162	0.813	0.189	0.228	14.576	0.867	0.101	0.014	0.042	0.016	0.016	1.056
11....	16.413	0.565	0.266	1.131	0.079	0.549	19.003	1.173	0.061	0.017	0.047	0.008	0.059	1.363
12....	0.458	0.244	0.157	0.240	0.042	0.281	1.422	0.053	0.029	0.012	0.018	0.004	0.034	0.150
13....	0.328	0.685	0.303	0.149	0.091	0.429	1.985	0.037	0.085	0.022	0.013	0.011	0.048	0.215
14....	3.296	0.174	0.119	0.190	0.055	0.149	3.982	0.242	0.017	0.009	0.014	0.005	0.013	0.300
15....	4.482	0.298	0.133	0.536	0.081	0.360	5.890	0.316	0.036	0.009	0.042	0.008	0.035	0.447
16....	0.935	0.437	0.288	0.141	0.087	0.442	2.327	0.154	0.069	0.023	0.011	0.009	0.089	0.315
MEAN....	3.824	0.980	0.657	0.441	0.129	0.505	8.536	0.303	0.089	0.037	0.030	0.010	0.044	0.502

RECEPTOR NUMBER	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
1.....	0.000	0.176	0.007	0.718	0.323	0.017	1.242	0.000	0.015	0.000	0.057	0.022	0.001	0.095
2.....	0.000	0.185	0.105	0.674	0.279	0.000	1.243	0.000	0.015	0.004	0.033	0.017	0.000	0.069
3.....	0.904	2.341	1.457	2.664	0.277	1.188	8.831	0.083	0.200	0.044	0.208	0.021	0.081	0.635
4.....	0.844	2.311	0.766	1.525	0.213	0.010	5.669	0.074	0.202	0.036	0.102	0.018	0.001	0.433
5.....	0.172	0.348	0.285	1.268	0.084	0.001	2.135	0.014	0.029	0.013	0.076	0.005	0.000	0.137
6.....	7.048	1.835	1.447	2.290	0.097	2.911	15.628	0.501	0.176	0.062	0.152	0.008	0.187	1.088
7.....	4.120	1.362	0.005	0.630	0.136	0.001	6.254	0.308	0.107	0.000	0.034	0.008	0.000	0.457
8.....	1.661	0.209	0.025	1.412	0.064	0.029	3.400	0.146	0.019	0.001	0.094	0.004	0.002	0.267
9.....	0.472	1.889	1.093	1.043	0.047	0.049	4.592	0.040	0.192	0.053	0.082	0.003	0.003	0.373
10....	7.342	0.064	0.025	0.543	0.666	0.000	8.640	0.519	0.005	0.001	0.032	0.045	0.000	0.602
11....	9.980	1.083	0.238	1.209	0.069	2.685	15.265	0.703	0.089	0.008	0.099	0.004	0.208	1.111
12....	0.452	0.251	0.015	2.492	0.007	0.111	3.328	0.039	0.025	0.001	0.161	0.001	0.008	0.234
13....	0.248	3.010	0.330	1.372	0.890	0.249	6.099	0.022	0.261	0.011	0.096	0.074	0.019	0.483
14....	2.086	0.318	0.070	1.518	0.325	0.001	4.318	0.152	0.026	0.003	0.093	0.022	0.000	0.295
15....	2.702	0.876	0.006	3.362	0.086	0.043	7.075	0.191	0.077	0.000	0.226	0.007	0.003	0.504
16....	0.081	0.907	0.568	0.710	0.257	2.424	4.946	0.010	0.086	0.024	0.041	0.019	0.215	0.395
MEAN....	2.382	1.073	0.403	1.484	0.237	0.607	5.167	0.175	0.095	0.016	0.099	0.017	0.048	0.449

RECEPTOR NUMBER	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
1.....	0.000	0.042	0.014	1.729	0.289	0.004	2.078	0.000	0.004	0.001	0.153	0.021	0.000	0.178
2.....	0.000	0.081	0.236	0.639	0.726	0.000	1.683	0.000	0.007	0.009	0.037	0.047	0.000	0.100
3.....	7.375	5.816	3.721	7.193	0.693	3.566	28.364	0.678	0.517	0.123	0.599	0.055	0.258	2.231
4.....	7.147	5.823	4.463	2.520	0.235	0.001	20.188	0.700	0.534	0.251	0.196	0.021	0.000	1.701
5.....	1.387	0.516	2.635	2.035	0.071	0.024	6.668	0.121	0.044	0.137	0.141	0.006	0.002	0.450
6.....	30.671	4.704	5.499	4.913	0.264	6.796	52.847	2.233	0.478	0.289	0.391	0.026	0.455	3.872
7.....	20.975	2.383	0.006	1.188	0.127	0.041	24.720	1.627	0.189	0.000	0.055	0.008	0.003	1.882
8.....	13.768	0.485	0.037	3.048	0.087	0.315	17.740	1.284	0.044	0.002	0.209	0.006	0.023	1.568
9.....	3.925	5.533	4.168	3.672	0.117	0.763	18.179	0.364	0.590	0.212	0.311	0.008	0.054	1.538
10....	32.385	0.104	0.050	1.310	1.503	0.000	35.353	2.354	0.008	0.003	0.084	0.105	0.000	2.553
11....	43.558	2.132	1.402	2.072	0.048	7.438	56.650	3.142	0.190	0.051	0.173	0.003	0.629	4.188
12....	3.739	0.362	0.014	3.786	0.002	0.040	7.944	0.349	0.039	0.001	0.246	0.000	0.003	0.638
13....	2.083	7.397	2.113	2.307	1.842	1.609	17.332	0.191	0.671	0.079	0.188	0.182	0.139	1.430
14....	9.927	0.160	0.443	2.584	0.950	0.009	14.073	0.743	0.013	0.019	0.171	0.068	0.001	1.015
15....	11.557	1.399	0.010	6.539	0.057	0.066	19.627	0.825	0.130	0.001	0.480	0.006	0.006	1.444
16....	0.741	2.453	2.293	1.824	0.460	7.982	15.754	0.091	0.252	0.109	0.121	0.037	0.790	1.400
MEAN....	11.826	2.462	1.684	2.980	0.467	1.791	21.200	0.919	0.232	0.080	0.222	0.036	0.148	1.637

Table 6. SO_2 and SO_4 source class contributions from PEM using hypothetical meteorology (8 consecutive 45 degree shifts in wind direction). Top: stability A; Middle: stability D; Bottom: stability E.

Stability Category	Wind Speed	Percent Contribution						
		area-coarse	area-fine	oil-ind	NJ-misc	grain	oil-misc	other
A	2 m/s	84.1	12.6	0.8	0.5	0.1	0.3	1.6
D	4	60.9	9.1	2.6	18.2	4.5	1.1	3.6
E	3	70.4	10.5	1.5	13.0	2.2	0.5	1.9

Table 7. Average (16 receptor) percent TSP source contributions from PEM modeling using hypothetical meteorology. Source classes contributing less than 1 percent of total TSP are labeled "other," and include refineries, coal, steel, chemical and soil.

Stability Category	Wind Speed	Percent Contribution					
		area	oil-ind	coal	oil-misc	chemical	refineries
A	2 m/s	60.4	17.7	5.4	6.0	2.0	8.8
D	4	39.0	21.2	3.6	22.0	3.8	10.0
E	3	56.1	14.2	4.9	13.6	2.2	9.0

Table 8. Average (16 receptor) percent SO_4 source class contributions from PEM modeling using hypothetical meteorology.

Actual Meteorology

Actual meteorological data were used to simulate three consecutive 12 hour periods, starting with 6 AM, August 22, 1982 (Table 9). These periods were selected since they showed diversity: transition from unstable daytime conditions to stability E (period 1); transition to stability A with some moderate and fairly persistent winds in categories B and C (period 2); neutral stability and low winds (period 3). Wind speed, direction, stability, and temperature data were complete for these periods.

Source class apportionments for TSP, SO_2 and SO_4 are shown in Tables 10 and 11. It is seen that area sources dominate as before, but other source classes may be significant contributors to both TSP and SO_4 concentrations. According to the source class inventory (Tables 2 and 3), area sources emit nearly one-half of the TSP within the city area. This is reflected in the source apportionment of Table 10.

Coal burning is the largest SO_2 emission class, and industrial oil burning produces most of the primary sulfate. In the vicinity of the city, however, most SO_2 and SO_4 is emitted by 6 industrial oil users and 4 refineries located near the city. The highest SO_2 and SO_4 concentrations from these sources (refineries) were 11.4 and 1.4 ug/m^3, respectively, for receptor 9 and period 1. These point sources have elevated stacks ranging from 40 to 84 m which generally result in low ground level concentrations. Consequently, area source emissions also dominated the source apportionment of SO_2 and SO_4.

The highest predicted sulfate concentration in the three periods was 6.3 ug/m^3 (receptor 11, period 1). A search for conditions that produced the maximum sulfate concentrations was performed by calculating hourly concentrations using the coarse grid with incremental 30 degrees shifts of wind direction under stability D for the receptors located in the city (Table 12). The maximum concentrations from point sources are considerably smaller than the average area source contributions. Only in one circumstance was the point source contribution roughly comparable to the area source contribution (receptor 10, wind direction 310 degrees, with an area source contribution of 1.016 ug/m^3 and an industrial oil source contribution of 0.588 ug/m^3). These results imply that most point sources contribute little to sulfate levels in the city under most conditions.

SCENARIO NUMBER	STABILITY CLASS	WIND SPEED CLASS	WIND SPEED (M/S)	WIND SECTOR	WIND DIRECTION (DEG)	AMBIENT TEMPERATURE (DEG C)
1	A		1.000		338.00	26.00
2	B		1.000		358.00	26.00
3	C		1.000		266.00	25.00
4	DD		1.000		276.00	25.00
5	DD		1.000		279.00	24.00
6	DN		1.000		282.00	23.00
7	E		1.000		340.00	22.00
8	E		1.000		284.00	22.00
9	DN		1.000		312.00	21.00
10	E		1.000		36.00	21.00
11	E		1.000		262.00	19.00
12	E		1.000		257.00	19.00

SCENARIO NUMBER	STABILITY CLASS	WIND SPEED CLASS	WIND SPEED (M/S)	WIND SECTOR	WIND DIRECTION (DEG)	AMBIENT TEMPERATURE (DEG C)
1	DN		1.000		244.00	19.00
2	DD		1.000		284.00	21.00
3	DD		1.500		40.00	24.00
4	C		2.300		62.00	25.00
5	B		2.500		66.00	26.00
6	C		2.800		56.00	27.00
7	B		2.200		57.00	26.00
8	B		1.900		88.00	27.00
9	A		1.900		49.00	26.00
10	A		1.400		313.00	28.00
11	A		1.700		77.00	28.00
12	A		1.100		109.00	28.00

Table 9. Meteorological data used for PEM simulation. All mixing heights set to 2000 m and inversion penetration factor set to unity. Top: period 1; bottom; period 2.

SCENARIO NUMBER	STABILITY CLASS	WIND SPEED CLASS	WIND SPEED (M/S)	WIND SECTOR	WIND DIRECTION (DEG)	AMBIENT TEMPERATURE (DEG C)
1	A		1.300		354.00	28.00
2	B		1.100		323.00	26.00
3	C		1.200		17.00	24.00
4	DD		1.200		108.00	23.00
5	DD		1.400		187.00	23.00
6	DD		1.000		173.00	22.00
7	DD		1.300		305.00	22.00
8	DD		1.000		219.00	21.00
9	DD		1.000		309.00	20.00
10	DD		1.000		284.00	19.00
11	DN		1.000		147.00	18.00
12	E		1.000		93.00	17.00

Table 9. (continued) Meteorological data; period 3.

RECEPTOR NUMBER	SOURCE CLASS CONTRIBUTION IN UG/M3												TOTAL
	AREA-C	AREA-F	REFIN.	INCIN.	OIL-IND	COAL	STEEL	NU-MIS	CHEM.	GRAIN	SOIL	OIL-MIS	CONCENT
1.....	12.141	1.789	0.018	0.000	1.070	0.144	0.026	0.000	0.108	0.000	0.000	0.074	15.350
2.....	6.577	0.826	0.000	0.034	0.001	0.045	0.005	0.000	0.000	0.000	0.000	0.013	7.501
3.....	0.000	0.000	0.000	0.000	0.000	0.447	0.502	0.000	0.000	0.000	0.000	0.014	0.963
4.....	0.000	0.000	0.000	0.000	0.247	0.181	0.016	0.000	0.008	0.000	0.000	0.000	0.453
5.....	21.581	3.344	0.084	0.016	0.276	0.340	0.376	0.000	0.065	0.003	3.410	0.251	29.745
6.....	214.910	33.108	0.003	0.002	0.044	0.048	0.080	0.026	0.005	0.000	0.000	0.031	248.257
7.....	153.250	19.257	0.000	0.008	0.013	1.003	0.492	0.000	0.027	0.000	0.000	0.043	174.093
8.....	0.000	0.000	0.000	0.000	1.451	1.537	0.070	0.000	0.050	0.000	0.000	0.154	3.263
9.....	15.197	2.198	0.119	0.003	0.060	0.263	0.000	1.977	0.097	4.833	2.863	0.215	27.825
10....	185.170	27.876	0.066	0.003	0.005	0.063	0.022	2.735	0.013	0.220	0.348	0.246	216.766
11....	298.450	47.321	0.004	0.017	0.032	0.540	0.036	0.224	0.063	0.000	0.000	0.116	346.804
12....	0.000	0.000	0.001	0.003	0.079	2.253	3.648	0.000	0.322	0.000	0.083	0.023	6.413
13....	10.639	1.629	0.313	0.034	0.073	0.083	0.010	0.001	0.012	0.007	3.139	0.075	16.015
14....	47.240	7.188	0.169	0.003	0.334	0.176	0.014	6.076	0.107	11.832	0.829	0.429	74.197
15....	111.480	16.376	0.007	0.218	0.298	0.294	0.103	0.037	0.262	0.003	0.066	0.262	129.404
16....	0.000	0.000	0.003	0.007	0.113	0.993	0.054	3.493	1.013	0.001	0.000	0.033	5.711
MEAN....	67.290	10.056	0.049	0.022	0.256	0.526	0.341	0.911	0.135	1.056	0.659	0.124	81.422

RECEPTOR NUMBER	SOURCE CLASS CONTRIBUTION IN UG/M3												TOTAL
	AREA-C	AREA-F	REFIN.	INCIN.	OIL-IND	COAL	STEEL	NU-MIS	CHEM.	GRAIN	SOIL	OIL-MIS	CONCENT
1.....	4.640	0.711	0.505	0.082	0.205	0.095	0.015	0.082	0.061	0.579	0.102	0.193	7.251
2.....	4.963	0.716	0.119	0.076	0.068	0.037	0.006	0.137	0.128	0.039	0.023	0.122	6.433
3.....	2.276	0.313	0.003	0.049	0.316	0.038	0.006	0.177	0.040	0.000	0.013	0.045	3.278
4.....	0.816	0.124	0.002	0.007	0.001	0.006	0.005	0.113	0.013	0.000	0.004	0.009	1.101
5.....	6.750	0.989	0.547	0.008	0.080	0.090	0.024	0.442	0.025	0.001	1.167	0.082	10.203
6.....	69.404	10.664	0.041	0.155	0.642	0.030	0.089	1.047	0.189	0.011	0.373	0.186	82.830
7.....	51.098	6.509	0.005	0.060	0.032	0.057	0.030	0.160	0.057	0.000	0.026	0.100	58.134
8.....	0.088	0.012	0.003	0.000	0.000	0.016	0.000	0.226	0.008	0.000	0.000	0.010	0.365
9.....	5.594	0.870	0.149	0.002	0.067	0.073	0.002	2.378	0.011	0.037	0.000	0.043	9.227
10....	50.321	7.565	0.019	0.009	0.124	0.022	0.016	0.483	0.076	19.737	0.021	0.020	78.413
11....	88.269	14.211	0.012	0.000	0.001	0.022	0.001	1.852	0.028	0.000	0.006	0.042	104.448
12....	0.000	0.000	0.000	0.000	0.000	0.069	0.004	0.169	0.013	0.000	0.001	0.029	0.285
13....	1.391	0.191	0.001	0.007	0.073	0.005	0.009	0.149	0.007	0.031	0.001	0.009	1.874
14....	3.332	0.502	0.000	0.025	0.010	0.044	0.008	0.427	0.007	0.000	0.069	0.012	4.438
15....	19.372	2.749	0.014	0.000	0.482	0.030	0.006	0.096	0.199	0.001	13.685	0.026	36.861
16....	0.000	0.000	0.000	0.000	0.000	0.058	0.000	3.311	0.026	0.000	0.000	0.030	3.425
MEAN....	19.270	2.883	0.089	0.030	0.131	0.043	0.014	0.702	0.056	1.277	0.968	0.060	25.822

RECEPTOR NUMBER	SOURCE CLASS CONTRIBUTION IN UG/M3												TOTAL
	AREA-C	AREA-F	REFIN.	INCIN.	OIL-IND	COAL	STEEL	NU-MIS	CHEM.	GRAIN	SOIL	OIL-MIS	CONCENT
1.....	0.233	0.029	0.000	0.014	0.053	0.034	0.008	3.048	0.010	0.000	0.000	0.004	3.431
2.....	12.268	1.880	0.000	0.002	0.179	0.045	0.011	4.238	0.093	0.819	0.051	0.043	19.629
3.....	18.364	2.661	0.004	0.150	0.194	0.051	0.011	7.662	0.092	0.000	0.413	0.223	29.825
4.....	5.733	0.809	0.000	0.000	0.000	0.020	0.045	0.143	0.388	2.882	0.115	0.085	10.219
5.....	1.766	0.270	0.005	0.032	0.196	0.120	0.009	6.070	0.064	0.458	0.000	0.042	9.032
6.....	117.300	18.076	0.000	0.005	0.102	0.023	0.018	6.561	0.029	0.000	0.009	0.020	142.145
7.....	105.810	13.929	0.002	0.080	0.176	0.063	0.035	0.087	0.017	3.968	1.620	0.085	125.851
8.....	10.422	1.560	0.002	0.000	0.007	0.030	0.046	0.474	0.408	3.015	0.396	0.084	16.446
9.....	3.315	0.510	0.112	0.050	0.114	0.121	0.024	8.966	0.037	0.684	0.136	0.095	14.164
10....	80.783	12.050	0.000	0.030	0.139	0.078	0.043	19.369	0.058	0.000	2.548	0.051	115.150
11....	160.780	25.843	0.000	0.000	0.693	0.010	0.001	2.901	0.000	3.313	1.058	0.003	194.402
12....	8.191	1.249	0.000	0.000	0.208	0.065	0.025	2.588	0.283	0.014	2.458	0.076	19.156
13....	2.330	0.328	0.001	0.026	0.068	0.001	0.016	8.060	0.014	0.030	0.019	0.044	10.938
14....	4.840	0.759	0.000	0.037	0.276	0.041	0.003	0.629	0.016	0.000	0.755	0.031	7.378
15....	33.367	4.721	0.000	0.000	0.003	0.002	0.006	4.625	0.000	0.000	0.230	0.013	42.966
16....	3.988	0.615	0.001	0.000	0.063	0.051	0.014	0.561	0.029	1.144	1.814	0.006	8.286
MEAN....	35.593	5.331	0.008	0.027	0.154	0.047	0.020	4.747	0.098	1.020	0.727	0.056	47.826

Table 10. TSP source class contributions using actual meteorology. Top--period 1; middle--period 2; bottom--period 3.

RECEPTOR NUMBER	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
1.....	2.808	1.863	0.771	0.859	1.246	1.560	9.107	0.374	0.281	0.090	0.102	0.172	0.117	1.136
2.....	1.047	0.010	0.011	0.150	0.000	0.003	1.222	0.127	0.001	0.001	0.013	0.000	0.000	0.143
3.....	2.789	0.000	0.092	0.191	0.000	0.000	3.072	0.456	0.000	0.008	0.046	0.000	0.000	0.509
4.....	2.234	0.320	0.217	0.003	0.079	0.000	2.853	0.345	0.036	0.013	0.001	0.008	0.000	0.402
5.....	6.692	3.037	0.290	2.869	0.730	6.505	20.123	0.910	0.452	0.019	0.374	0.095	0.658	2.508
6.....	58.654	0.486	0.148	0.352	0.061	0.089	59.789	4.652	0.053	0.010	0.033	0.006	0.011	4.765
7.....	27.610	0.158	0.209	0.418	0.265	0.011	28.671	2.161	0.014	0.023	0.084	0.033	0.002	2.317
8.....	4.414	2.322	1.331	1.505	0.521	0.000	10.093	0.602	0.308	0.117	0.298	0.056	0.000	1.381
9.....	6.345	0.634	0.386	0.714	1.048	11.071	20.199	0.895	0.091	0.033	0.117	0.134	1.440	2.710
10....	66.185	0.056	0.050	2.913	0.106	0.438	69.748	5.405	0.008	0.006	0.217	0.009	0.041	5.685
11....	79.630	0.370	0.152	1.310	0.733	0.068	82.264	6.050	0.045	0.021	0.133	0.072	0.012	6.332
12....	1.200	0.258	2.473	0.318	1.865	0.015	6.129	0.161	0.038	0.428	0.068	0.210	0.003	0.908
13....	2.266	0.737	0.606	0.801	0.141	9.869	14.420	0.308	0.122	0.064	0.148	0.018	1.525	2.183
14....	26.885	3.768	0.281	2.794	0.167	1.238	35.133	2.698	0.456	0.035	0.281	0.020	0.166	3.656
15....	32.090	0.681	0.273	3.014	3.007	0.057	39.122	2.916	0.117	0.040	0.296	0.376	0.009	3.754
16....	0.745	0.955	0.281	0.418	2.256	0.050	4.704	0.194	0.153	0.048	0.048	0.327	0.011	0.783
MEAN....	20.100	0.979	0.473	1.184	0.764	1.936	25.416	1.766	0.136	0.060	0.141	0.098	0.250	2.448

RECEPTOR NUMBER	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
1.....	0.284	2.288	0.815	2.112	0.283	2.864	8.647	0.035	0.203	0.015	0.168	0.024	0.203	0.648
2.....	0.654	0.702	0.236	1.342	1.295	0.658	4.887	0.071	0.070	0.022	0.100	0.118	0.062	0.443
3.....	2.650	2.438	0.232	0.534	0.167	0.005	6.026	0.345	0.212	0.026	0.041	0.018	0.001	0.641
4.....	2.042	0.004	0.098	0.091	0.018	0.003	2.255	0.305	0.001	0.011	0.012	0.003	0.000	0.331
5.....	0.341	0.706	0.177	0.916	0.011	2.661	4.812	0.040	0.092	0.018	0.066	0.001	0.163	0.381
6.....	18.478	8.812	0.506	2.130	1.488	0.183	29.598	1.445	0.553	0.042	0.131	0.092	0.012	2.274
7.....	10.720	0.097	0.144	1.077	0.466	0.007	12.511	0.900	0.011	0.013	0.068	0.039	0.001	1.033
8.....	3.702	0.000	0.127	0.094	0.001	0.003	3.928	0.488	0.000	0.012	0.011	0.000	0.000	0.512
9.....	0.532	0.158	0.101	0.244	0.031	0.781	1.845	0.067	0.027	0.013	0.026	0.003	0.053	0.190
10....	18.231	1.038	0.376	0.178	0.110	0.025	19.958	1.366	0.099	0.028	0.010	0.012	0.002	1.517
11....	25.114	0.002	0.431	0.293	0.106	0.016	25.962	1.855	0.000	0.028	0.027	0.008	0.001	1.919
12....	1.026	0.000	0.191	0.305	0.000	0.000	1.523	0.135	0.000	0.018	0.025	0.000	0.000	0.178
13....	0.290	0.412	0.034	0.099	0.078	0.008	0.920	0.036	0.062	0.005	0.010	0.011	0.001	0.126
14....	4.810	0.034	0.068	0.087	0.030	0.000	5.028	0.359	0.005	0.007	0.007	0.003	0.000	0.381
15....	6.769	5.404	1.053	0.236	0.001	0.019	13.482	0.491	0.588	0.051	0.019	0.000	0.001	1.150
16....	0.433	0.000	0.274	0.042	0.001	0.000	0.749	0.075	0.000	0.018	0.005	0.000	0.000	0.098
MEAN....	6.005	1.256	0.304	0.611	0.255	0.452	8.883	0.501	0.120	0.020	0.045	0.021	0.031	0.739

RECEPTOR NUMBER	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
1.....	0.000	0.499	0.016	0.053	0.028	0.000	0.596	0.000	0.065	0.002	0.008	0.004	0.000	0.078
2.....	3.557	0.573	0.115	0.508	0.302	0.000	5.056	0.472	0.070	0.012	0.038	0.031	0.000	0.623
3.....	5.830	0.280	0.157	2.542	0.857	0.005	9.671	0.858	0.039	0.013	0.314	0.116	0.001	1.342
4.....	2.344	0.000	0.090	0.889	0.000	0.000	3.323	0.335	0.000	0.016	0.126	0.000	0.000	0.477
5.....	0.519	0.927	0.120	0.482	0.498	0.031	2.577	0.081	0.114	0.018	0.044	0.055	0.002	0.314
6.....	33.425	0.497	0.056	0.243	0.129	0.000	34.351	2.648	0.062	0.007	0.015	0.013	0.000	2.746
7.....	20.112	1.970	0.013	0.992	0.190	0.002	23.279	1.730	0.232	0.001	0.086	0.018	0.000	2.069
8.....	4.625	0.081	0.094	0.960	0.020	0.047	5.828	0.596	0.012	0.017	0.109	0.002	0.006	0.742
9.....	1.312	0.946	0.051	1.116	0.410	0.568	4.403	0.185	0.133	0.008	0.118	0.048	0.040	0.532
10....	32.478	1.584	0.027	0.602	0.659	0.000	35.351	2.444	0.142	0.004	0.042	0.069	0.000	2.702
11....	44.700	7.900	0.002	0.026	0.003	0.000	52.632	3.352	0.719	0.000	0.004	0.001	0.000	4.075
12....	1.432	2.316	0.033	0.888	0.015	0.002	4.685	0.181	0.297	0.005	0.068	0.002	0.000	0.554
13....	0.916	0.513	0.019	0.506	0.142	0.001	2.098	0.128	0.077	0.003	0.057	0.021	0.000	0.287
14....	9.187	3.099	0.009	0.241	0.184	0.000	12.721	0.731	0.349	0.002	0.025	0.018	0.000	1.123
15....	12.803	0.003	0.002	0.142	0.001	0.000	12.952	0.983	0.001	0.000	0.014	0.000	0.000	0.998
16....	1.389	0.707	0.020	0.064	0.005	0.007	2.193	0.256	0.089	0.004	0.007	0.001	0.001	0.357
MEAN....	10.914	1.389	0.051	0.641	0.215	0.042	13.232	0.936	0.150	0.007	0.067	0.025	0.003	1.188

Table 11. SO_2 and SO_4 source class contributions using actual meteorology. Top--period 1; middle--period 2; bottom--period 3.

Table 12 also shows that area source contributions remain constant under varying wind directions. According to this modeling, only the area source in which the receptor resides is an important contributor to sulfate. Note however, that the relatively large receptor grid size of 10 km encompasses 16 of the 2.5 area sources. This results in less variation than might be found with smaller grid sizes.

The PEM results support the observation in Section 3 that secondary sulfate may compose a large fraction of the sulfate mass, especially from distant sources. Sulfate may attain about 10 percent of the SO_2 mass, although only 4.3 percent primary sulfate is emitted by all sources. However, it should be recalled that the SO_4 emission factor for area sources was 7 percent. (A molecular weight ratio of 1.5 (SO_4/SO_2) was used for mass conversion.)

DISCUSSION

PEM modeling of the Philadelphia area is constrained by the limited accuracy of the source inventory. In particular, estimates of area source emissions, which dominated the apportionment, are very crude. More accurate modeling may require better inventories, especially around receptor sites and more detailed meteorological data. The Norristown station does not necessarily provide representative surface observations for the Philadelphia area. Also, the omission of mixing height data will bias results. Mixing height was simply set to 2000 m. Lower mixing heights were found to alter point source contributions by up to 40 percent. Very low mixing heights (e.g., 200 m) eliminated point source contributions since elevated sources had plumes that penetrated the ceiling layer.

Using 9 monitoring sites in Philadelphia from May to September 1979, Suggs and Barton (1983) obtained 24 hour concentrations of fine particles ranging from 2 to 54 with a mean of 29 ug/m^3. TSP concentrations at the same sites ranged from 15 to 172 ug/m^3 with a mean of 56 ug/m^3. Predicted sulfate concentrations at the four receptors located within Philadelphia (numbers 6, 7, 10, 11) ranged from 0.5 to 6.3 ug/m^3 for the three 12 hour periods. The corresponding TSP predictions ranged from 58 to 346 ug/m^3.

	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
WIND ANGLE														
10....	14.002	0.000	0.000	0.008	0.000	0.000	14.007	1.014	0.000	0.000	0.000	0.000	0.000	1.015
40....	14.002	0.000	0.000	1.877	0.000	0.000	15.879	1.014	0.000	0.000	0.174	0.000	0.000	1.189
70....	14.002	3.205	0.000	0.072	0.000	0.000	17.280	1.014	0.320	0.000	0.003	0.000	0.000	1.338
100...	14.002	0.000	0.000	0.221	0.009	0.000	14.232	1.014	0.000	0.000	0.009	0.001	0.000	1.024
130...	14.002	0.000	0.000	0.000	0.000	0.002	14.004	1.014	0.000	0.000	0.000	0.000	0.000	1.015
160...	14.002	0.000	0.000	0.000	0.000	0.000	14.002	1.014	0.000	0.000	0.000	0.000	0.000	1.014
190...	14.002	0.000	0.000	0.000	0.000	0.000	14.002	1.014	0.000	0.000	0.000	0.000	0.000	1.014
220...	14.002	0.000	0.000	0.184	0.000	0.037	14.223	1.014	0.000	0.000	0.016	0.000	0.003	1.033
250...	14.002	0.000	0.000	0.000	0.000	0.000	14.002	1.014	0.000	0.000	0.000	0.000	0.000	1.014
280...	14.002	0.000	0.001	0.118	0.000	0.000	14.122	1.014	0.000	0.000	0.016	0.000	0.000	1.031
310...	14.002	1.022	0.728	0.342	0.158	0.000	16.251	1.014	0.125	0.051	0.049	0.017	0.000	1.257
340...	14.002	2.156	0.000	0.003	0.074	0.000	16.236	1.014	0.189	0.000	0.000	0.006	0.000	1.309

	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
WIND ANGLE														
10....	8.806	0.000	0.000	0.023	0.000	0.000	8.829	0.688	0.000	0.000	0.002	0.000	0.000	0.690
40....	8.806	0.000	0.000	0.000	0.000	0.000	8.806	0.688	0.000	0.000	0.000	0.000	0.000	0.688
70....	8.806	0.000	0.000	0.421	0.000	0.000	9.227	0.688	0.000	0.000	0.046	0.000	0.000	0.734
100...	8.806	0.231	0.000	0.293	0.000	0.000	9.330	0.688	0.023	0.000	0.026	0.000	0.000	0.737
130...	8.806	0.007	0.000	0.142	0.000	0.000	8.955	0.688	0.001	0.000	0.006	0.000	0.000	0.695
160...	8.806	0.008	0.000	0.121	0.232	0.355	9.522	0.688	0.001	0.000	0.009	0.015	0.028	0.740
190...	8.806	0.000	0.000	0.074	0.000	0.000	8.879	0.688	0.000	0.000	0.007	0.000	0.000	0.695
220...	8.806	0.998	0.000	0.000	0.028	0.160	9.992	0.688	0.111	0.000	0.000	0.002	0.015	0.816
250...	8.806	0.000	0.003	0.013	0.000	0.000	8.821	0.688	0.000	0.000	0.002	0.000	0.000	0.690
280...	8.806	0.284	0.547	0.030	0.163	0.000	9.829	0.688	0.022	0.033	0.003	0.015	0.000	0.760
310...	8.806	0.019	0.113	0.044	0.068	0.000	9.048	0.688	0.002	0.007	0.006	0.007	0.000	0.710
340...	8.806	0.000	0.000	0.335	0.000	0.000	9.140	0.688	0.000	0.000	0.033	0.000	0.000	0.721

	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
WIND ANGLE														
10....	14.158	0.095	0.000	0.031	0.000	0.000	14.284	1.016	0.008	0.000	0.002	0.000	0.000	1.026
40....	14.158	0.000	0.000	0.556	0.000	0.000	14.714	1.016	0.000	0.000	0.054	0.000	0.000	1.070
70....	14.158	0.000	0.000	0.000	0.000	0.000	14.158	1.016	0.000	0.000	0.000	0.000	0.000	1.016
100...	14.158	0.000	0.000	0.000	0.000	0.000	14.158	1.016	0.000	0.000	0.000	0.000	0.000	1.016
130...	14.158	0.000	0.000	0.000	0.000	0.000	14.158	1.016	0.000	0.000	0.000	0.000	0.000	1.016
160...	14.158	0.000	0.000	0.000	0.000	0.000	14.158	1.016	0.000	0.000	0.000	0.000	0.000	1.016
190...	14.158	0.000	0.000	0.000	0.000	0.000	14.158	1.016	0.000	0.000	0.000	0.000	0.000	1.016
220...	14.158	0.000	0.000	0.000	0.000	0.000	14.158	1.016	0.000	0.000	0.000	0.000	0.000	1.016
250...	14.158	1.031	0.000	0.615	0.028	0.029	15.861	1.016	0.118	0.000	0.063	0.003	0.003	1.202
280...	14.158	0.000	0.004	0.039	0.115	0.000	14.316	1.016	0.000	0.000	0.006	0.007	0.000	1.030
310...	14.158	5.448	1.295	0.640	0.841	0.000	22.382	1.016	0.588	0.102	0.098	0.086	0.000	1.890
340...	14.158	0.000	0.000	0.282	0.000	0.000	14.440	1.016	0.000	0.000	0.025	0.000	0.000	1.041

	- - - SO2 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -							- - - SO4 SOURCE CLASS CONTRIBUTIONS IN UG/M3 - - -						
	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL	AREA	OIL-IND	COAL	OIL-MIS	CHEM.	REFIN.	TOTAL
WIND ANGLE														
10....	20.108	0.000	0.000	0.000	0.000	0.000	20.108	1.448	0.000	0.000	0.000	0.000	0.000	1.448
40....	20.108	0.000	0.000	0.752	0.000	0.000	20.860	1.448	0.000	0.000	0.064	0.000	0.000	1.511
70....	20.108	0.000	0.000	0.012	0.000	0.000	20.120	1.448	0.000	0.000	0.001	0.000	0.000	1.449
100...	20.108	0.000	0.000	0.000	0.000	0.000	20.108	1.448	0.000	0.000	0.000	0.000	0.000	1.448
130...	20.108	0.000	0.000	0.000	0.000	0.000	20.108	1.448	0.000	0.000	0.000	0.000	0.000	1.448
160...	20.108	2.518	0.000	0.000	0.000	0.000	22.626	1.448	0.202	0.000	0.000	0.000	0.000	1.650
190...	20.108	0.000	0.000	3.784	0.049	0.373	24.314	1.448	0.000	0.000	0.184	0.004	0.029	1.644
220...	20.108	0.010	0.000	0.878	0.628	0.300	21.919	1.448	0.001	0.000	0.091	0.044	0.032	1.615
250...	20.108	0.000	0.000	0.014	0.000	0.000	20.122	1.448	0.000	0.000	0.001	0.000	0.000	1.448
280...	20.108	0.930	0.358	0.129	0.572	0.000	22.096	1.448	0.085	0.027	0.008	0.061	0.000	1.628
310...	20.108	0.000	0.000	0.015	0.000	0.000	20.123	1.448	0.000	0.000	0.002	0.000	0.000	1.449
340...	20.108	0.000	0.000	0.000	0.000	0.000	20.108	1.448	0.000	0.000	0.000	0.000	0.000	1.448

Table 12. Apportionment of hourly SO_2 and SO_4 concentrations (in ug/m^3) at four city receptors. Top to bottom: receptors 6, 7, 10 and 11.

Thus, PEM predictions have the correct order of magnitude, although TSP predictions seem high, and sulfate seem low. However, observed particle concentrations include non-sulfate species as well as background regional levels. Background concentrations were not included in the PEM modeling.

SECTION 4

RECEPTOR MODELS

The principal objectives of this section include the following:

(1) Brief review of receptor models (RMs);

(2) Application and evaluation of several diagnostic procedures designed to minimize the spurious results obtained by chemical mass balance RMs, and suggestions for protocols which incorporate these diagnostic tools;

(3) Suggestions for the development and application of hybrid models, i.e., models which combine aspects of dispersion and receptor models;

(4) Description of issues concerning inter-comparisons between results of receptor and dispersion models;

(5) Discussion of issues concerning RM protocols.

OVERVIEW OF RECEPTOR MODELS

Receptor models are procedures which use observed aerosol characteristics to identify and quantify the sources of ambient air pollutants. The aerosol characteristics most frequently measured include the chemical and elemental mass, optical properties and particle size distribution. Less frequently measured characteristics include isotope ratios, organic and inorganic compounds, and crystalline structure. Unlike dispersion models, RMs do not require meteorological or source data. Source profiles may be used, but are not necessary.

In general, RMs make use of the following assumptions:

Non-reactive (conservative) aerosols. The total aerosol mass at a receptor is a linear sum of the aerosol contributions from individual sources. In general, there can not be any transformation of the aerosol from time of emissions at the source through atmospheric transport to collection and ultimate analysis.

Stable aerosol characteristics. Characteristics of the aerosols are a linear sum of the aerosol characteristics from individual sources, e.g., elemental ratios are assumed to be constant between source and receptor.

Identifying aerosol characteristics for source classes. Source apportionment is possible only for those source classes that have identifying characteristics. No unique characteristic is needed: just a unique combination of characteristics.

Description of source profiles. Chemical mass balance models require quantification of source characteristics, e.g., elemental ratios. Multivariate models require less precise descriptions, but patterns of characteristics must be recognizable. Sources with unknown or highly variable characteristics may not be distinguishable.

Miscellaneous statistical assumptions. For regression models, the number of characteristics must exceed the number of source classes, and errors (residuals) should be normally distributed and uncorrelated. For multivariate models, the number of filters must be sufficient for the degrees of freedom required for the number of filter characteristics and sources used.

Deviations from these assumptions will degrade the validity of the receptor model. The magnitude of the deviations that typically occur in RM applications is not known at the present time. Also unknown is the susceptibility of RMs to such deviations. There are obvious situations where the assumptions are violated and RM applications may not be useful. For example, RM assumptions do not hold for secondary pollutants, e.g., smog or sulfate, which undergo extensive transformation and scavenging. Also, RMs can not apportion sources within a source category, e.g., determining which of two power plants is culpable, since these sources have similar aerosol characteristics.

There are many approaches to receptor modeling based on the above assumptions. Cooper (1980) has classified receptor models by the interpretive approach used to associate aerosol characteristics with emission sources. These approaches include 1) regression analysis of

aerosol characteristics, which has been labeled the chemical mass balance (CMB) approach; 2) multivariate analyses of the variability of aerosol characteristics; 3) composite receptor models which combine CMB and multivariate methods; and 4) a miscellaneous category including enrichment or depletion processes, trajectory analyses and, in general, hybrid dispersion/receptor models. Table 13 highlights some of the major differences between model approaches. ERT (1981) and Thurston (1983) provide reviews of current models. A compilation of recent work in receptor modeling is found in APCA (1982). Some aspects of the different models are discussed below.

Chemical Mass Balance Receptor Models

Most chemical mass balance (CMB) models minimize the sum of squared residuals (SSR) between observed and predicted aerosol characteristics:

$$\text{Minimize SSR} = (\underline{A}\,\underline{S} - \underline{C})^T (\underline{A}\,\underline{S} - \underline{C})$$

where: $\underline{A}$ is the vector of estimated source apportionment (a_i is the contribution of source class i to total pollutant mass).

$\underline{S}$ is the source profile matrix ($s_{i,j}$ is a measure of aerosol characteristic j emitted by source class i).

$\underline{C}$ is the vector of observed ambient characteristic (c_i is a measure of characteristic i).

CMB models require measured characteristics for one or more time periods and source profiles. Table 14 shows the source profiles for sources used in the Quail Roost II study of RMs. Ambient sampling and analysis procedures are quite sophisticated. However, source sampling involves greater practical difficulties and less accuracy. Moreover, source profiles often are unavailable or highly variable within source classes (e.g., from one oil burner to another), as well as dependent on operating conditions (e.g., fuel burned). Consequently, the matrix of source profiles, $\underline{S}$, may be very approximate. CMB models using inappropriate source profiles may produce

	Dispersion Models	------Receptor Models------		
		CMB	Multivariate	Composite
Identification of culpability				
Individual sources	X	-	-	-
Source classes	-	X	-	-
Combined source classes	-	-	X	X
Source apportionment				
Quantitative	X	X	-	X
Qualitative	-	-	X	-
Uncertainty estimates				
Quantitative	-	X	-	X
Qualitative	-	-	X	-
Data Requirements				
Source strength, location	X	-	-	-
Source profiles	-	X	-	X
Meteorology	X	-	-	-

Table 13. Differences between major classes of receptor and dispersion models.

	SOURCE CLASS												
	STEELA	STEELB	OILA	INCIN	OILB	COALA	AGGREG	GLASS	BASALT	SOIL	AUTO	WOOD	COALB
C.....	149158	214629	40617	39991	198625	30450	985	2036	150	68593	518497	575515	7045
NA.....	9263	14438	22526	132260	20676	8648	5235	158253	20158	4271	74649	3327	4459
AL.....	13198	10569	6947	4855	6088	29387	59713	3622	85596	186744	8320	8216	164018
SI.....	8995	11653	195753	7424	76428	142062	235758	1989	166164	435851	9308	7981	155397
S.....	24948	46829	135376	132183	123929	15888	6589	178681	226	229	8762	868	133869
CL.....	33141	36707	824	297407	13071	10460	806	3079	196	92	8717	10030	18979
K.....	10200	12810	748	248410	1329	10407	13520	32591	8580	10086	2714	9426	8047
CA.....	63410	52272	836	11073	10814	26048	41693	4428	45793	20306	11288	7769	35386
TI.....	1448	1143	757	1013	1100	2845	2793	336	7910	12629	7	19	9011
V.....	189	145	9289	25	691	140	65	1611	223	280	106	3	797
CR.....	2848	3089	227	890	431	348	60	3827	118	310	89	3	330
MN.....	15216	22968	117	360	118	280	906	253	1633	2030	598	20	248
FE.....	123383	154932	13315	5721	13300	18908	49930	9104	81767	99805	7043	1032	71642
NI.....	3072	2797	5297	93	50	187	32	1271	85	103	61	5	635
CU.....	2310	3970	655	4248	595	1313	580	432	98	181	3	3	380
ZN.....	28211	42955	356	21080	1126	2756	490	554	83	391	3248	617	688
AS.....	82	114	12	129	235	287	41	651	12	20	12	12	182
BR.....	91	146	27	831	399	160	12	17	1	10	38708	96	11
PB.....	7876	13008	811	16863	4123	2029	119	507	4	310	133622	100	1197

Table 14. Source signatures from Quail Roost II in ug/g.

large errors. These models also are prone to several statistical problems, which may lead to spurious results, due to the similarity between some source profiles and sensitivity to small changes or errors in the measured aerosol characteristics.

CMB models have some advantages over multivariate RMs since they are conceptually very simple, quantitative source estimates are derived, and only one filter sample is needed. They also have fairly high resolution (about 5 to 7 source classes). Lastly, regression packages are commonly available on many computers.

CMB models use any of the following procedures: ordinary least squares, weighted least squares, effective variance techniques, robust and ridge regression.

Multivariate Receptor Models

Multivariate receptor models use a time series of ambient observations and look for consistent relationships among aerosol characteristics. They are mathematically very complex. Multivariate models have the significant advantage of not requiring an explicit source profile matrix. Thus, they may be used when the identity or profile of likely sources is unknown. This advantage is somewhat offset since about 40 (Pace, 1983) to 50 (Thurston, 1983) ambient samples must be collected to provide robust results. Additionally, these models indicate the source types and the amount of variance explained by each, but not the actual apportionment. Multivariate models tend to have lower resolution than CMB models, distinguishing perhaps 3 to 5 sources.

Multivariate procedures include multivariate regression, factor analysis, cluster analysis and principal component analysis.

Composite Receptor Models

Composite regression/multivariate receptor models have the ability to provide quantitative estimates of source apportionment without a precise source profile matrix. For instance, target transformation factor analysis rotates and scales the factor axis (derived using factor analysis procedures and the observed source characteristic matrix) such that the overlap with

estimated source profiles is maximized. Then, conventional CMB procedures are used to calculate mass contributions. This procedure may provide useful results when source profiles are not known a priori.

In addition to target transformation factor analysis, composite receptor models include multiple linear regression/factor analysis and effective variance CMB/factor analysis procedures.

DIAGNOSTIC PROCEDURES FOR CMB MODELS

This section discusses several problems which are frequently encountered in CMB receptor models. These problems are collinearity, influential characteristics and outliers. In part, the reliability and quantitative performance of CMB receptor modeling depend on resolving these problems. Some relatively new diagnostic procedures, which have not been applied previously (at least not in our search of the literature) are discussed and demonstrated. These procedures are developed in depth by Belsley, Kuh and Welsch (1980) and are implemented in the TROLL statistical package (Information Processing Service, 1980).

Collinearity

Collinearity exists when source profiles, e.g., elemental ratios, are similar or linearly dependent. In CMB models, collinearity may result from 1) similar source signatures; 2) too many source classes, and 3) too few observations, e.g., not enough elemental measures. In general, collinearity may lead to unstable, negative and/or too large estimates of source contributions from one or more source classes. Ordinary least squares (OLS) in CMB models can not be rationally applied before such dependencies have been established.

There are many diagnostic tools which may detect the presence of collinearity. These include:

-eigensystem analysis and condition number

-singular value decomposition and variance decomposition proportions

-examination of the correlation matrix of the source signatures

-variance inflation factor

These methods, which use only the source profile S (not the observations of

aerosol characteristics), are illustrated using the (contaminated) source profile matrix given to the Quail Roost II participants. This matrix (Table 14) contains 13 source profiles, each consisting of 19 elements. (The matrix was contaminated in Quail Roost II by adding random measurement errors to each element of the true source matrix.)

The singular value decomposition (SVD) and variance decomposition proportions (VDP) analyses are performed using the procedures of Belsley, et.al. (1980). The SVD consists of the first three columns of Table 15, where "rows" (1st column) correspond to eigenvectors of the source profile matrix, ranked by decreasing "singular values" (2nd column); and "condition indices" (3rd column) are the ratio of the largest singular value to the singular value of each row. (This analysis is similar to eigensystem analysis: singular values are the square roots of the eigenvalues, but are computed in a way which decomposes the source matrix $\underline{S}$, rather than $\underline{S}^T\underline{S}$.) The remaining columns show the VDP, where "coef" represents the 13 source profiles. The VDP, which range from 0 to 1 and sum to 1 in each column, show the fraction of variance associated with each source class and each eigenvector.

Collinearity which may be serious enough to degrade source apportionments is indicated by singular values with high condition indices (greater than about 100) and two or more high VDPs (greater than about 0.8 or 0.9). Table 15 clearly shows the dependence between oil-A and oil-B sources (condition index 122, coefficients 3 and 5) and a somewhat surprising multiple dependence between steel-A, steel-B, glass, basalt, and soil sources (condition index 300, coefficients 1, 2, 8, 9, and 10). The coefficients for these source classes may be poorly estimated by OLS regressions.

Somewhat similar dependencies for the Quail Roost II profiles are shown by the correlation matrix (Table 16). Very high or low correlations (near $\pm$ 1) indicate strong dependencies between two sources. There are six pairs of profiles that have correlations above 0.9, namely, steel-A and steel-B (arguments 1 and 2); coal-A and aggregate (6 and 7); aggregate and glass (7 and 8); aggregate and basalt (7 and 9); basalt and soil (9 and 10) and auto and wood (11 and 12). Note that correlation coefficients do not show multiple dependencies.

The variance inflation factor (VIF) does indicate both single and

PROPORTIONATE VARIANCE DECOMPOSITION MATRIX

ROW	SING.VAL.	COND.INDEX	COEF.1	COEF.2	COEF.3	COEF.4	COEF.5	COEF.6	COEF.7	COEF.8	COEF.9	COEF.10	COEF.11	COEF.12	COEF.13
1	2.9316	1.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2	1.82814	1.3848	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.003	0.	0.
3	1.25387	2.01904	0.	0.	0.	0.	0.033	0.	0.	0.003	0.	0.	0.	0.	0.
4	0.856041	2.95734	0.	0.	0.	0.	0.081	0.	0.	0.	0.	0.	0.002	0.	0.
5	0.720568	3.51335	0.	0.	0.	0.	0.122	0.	0.	0.002	0.	0.	0.003	0.	0.002
6	0.446701	5.66733	0.	0.	0.	0.	0.008	0.	0.	0.002	0.	0.	0.003	0.	0.034
7	0.413178	6.12718	0.	0.	0.002	0.	0.007	0.	0.	0.015	0.	0.	0.057	0.	0.001
8	0.181588	13.9415	0.	0.	0.003	0.	0.	0.	0.	0.01	0.	0.	0.62	0.025	0.008
9	0.135025	18.7491	0.001	0.003	0.008	0.025	0.001	0.008	0.	0.	0.	0.009	0.002	0.	0.015
10	0.044245	57.2177	0.	0.016	0.08	0.847	0.019	0.108	0.	0.101	0.069	0.008	0.059	0.001	0.14
11	0.027613	91.6814	0.014	0.024	0.021	0.014	0.125	0.075	0.299	0.013	0.014	0.068	0.093	0.22	0.42
12	0.020735	122.092	0.044	0.04	0.837	0.013	0.838	0.028	0.118	0.001	0.	0.003	0.051	0.834	0.321
13	0.008438	300.039	0.938	0.916	0.047	0.074	0.015	0.781	0.621	0.849	0.915	0.92	0.141	0.117	0.058

Table 15. Proportionate variance decomposition of the contaminated Quail Roost II source profiles. "Coef" correspond to 13 source class profiles (columns of Table 10. See Table 17 for identification of profile numbers.)

	ARG1	ARG2	ARG3	ARG4	ARG5	ARG6	ARG7	ARG8	ARG9	ARG10	ARG11	ARG12	ARG13
ARG1	1.000												
ARG2	0.985	1.000											
ARG3	0.048	0.097	1.000										
ARG4	0.014	0.024	0.040	1.000									
ARG5	0.407	0.488	0.400	0.108	1.000								
ARG6	0.136	0.124	0.822	-0.056	0.405	1.000							
ARG7	0.031	-0.002	0.749	-0.141	0.196	0.969	1.000						
ARG8	-0.060	-0.006	0.389	0.406	0.326	-0.036	-0.098	1.000					
ARG9	0.150	0.093	0.606	-0.182	0.117	0.877	0.946	-0.091	1.000				
ARG10	0.104	0.092	0.717	-0.177	0.286	0.951	0.965	-0.141	0.940	1.000			
ARG11	0.661	0.728	0.063	-0.013	0.764	0.084	-0.115	-0.024	-0.139	0.026	1.000		
ARG12	0.712	0.774	0.088	-0.006	0.802	0.123	-0.079	-0.088	-0.106	0.068	0.959	1.000	
ARG13	0.090	0.078	0.705	-0.009	0.327	0.681	0.706	0.259	0.769	0.747	-0.144	-0.096	1.000

Table 16. Simple correlation for the Quail Roost II source profiles. "Arg" numbers refer to source profiles. (See Table 17 for identification.)

-Number-	--Source--	--VIF--	-Number-	--Source--	--VIF--
1	Steel-A	2963	8	Glass	84
2	Steel-B	2258	9	Basalt	2320
3	Oil-A	728	10	Soil	2319
4	Incinerator	5	11	Automobile	23
5	Oil-B	1541	12	Wood	652
6	Coal-A	1646	13	Coal-B	108
7	Aggregate	2449			

Table 17. Variance inflation factors for the Quail Roost II source profiles.

multiple dependencies. The VIFs for the same profiles are shown in Table 17. A high VIF (above about 30) may indicate strong single or multiple dependencies. Table 17 suggests that a majority of the sources are involved in strong collinear relationships. However, the number of dependencies and the sources which contribute to them are not indicated by the VIFs.

We believe that the use of correlation coefficients and the singular value decomposition and variance decomposition procedure of the source profiles will provide a comprehensive identification of single and multiple dependencies. These procedures indicate the source classes which will be poorly estimated as well as those which are not adversely affected by the collinearity.

Remedial procedures for alleviating the problems caused by collinearity include:

-eliminating or combining sources

-using additional filter characteristics, e.g., more elemental analysis

-using ridge regression

-using principal components regression

Only the first procedure, eliminating (or combining) sources, is described here.

Eliminating sources from the CMB model is, perhaps, the simplest method of handling collinearity. The subset of sources to be used can be selected, in part, from the collinearity analysis. For the Quail Roost profiles, four or five of the collinear sources (e.g., oil-B, steel-A, glass and basalt) might be eliminated, based on the SVD and VDP analysis. However, it is necessary to account for the possibility that an actual source is eliminated in the CMB model. This is the problem of source selection, described below.

Source Selection

In Quail Roost II, the subset of sources for CMB modeling was selected as follows: 1) Initially, all sources were included in CMB modeling. 2) Sources with negative source contribution estimates were removed one at a time, discarding sources with the largest σ_i/a_i (uncertainty/estimated source contribution), and repeating CMB calculations for each removal. 3) When all source contribution estimates were positive, sources with the largest σ_i/a_i were removed, and the CMB calculations were repeated after

each removal. 4) After all σ_i/a_i were less than 1, discarded sources were added experimentally. This last step is necessary since this procedure does not necessarily guarantee the best model.

The "all possible regressions" (APR) procedure may provide a more rapid and systematic procedure of determining sources in CMB models. These computerized routines efficiently generate all possible regressions, that is, all possible combinations of sources (Montgomery and Peck, 1982). The procedure calculates regressions with 1 to p sources, where p may be specified by the user (and is less than or equal to n). For each level of p, the APR procedure calculates all regressions and determines the models with the best fits, then prints out the sources included in a specified number of the best models. This procedure is as fast as stepwise regression, and is less arbitrary in the sense that no combination of sources is omitted.

For n sources there are 2^n-1 possible regression models, a potentially large number. Practically, however, if strong collinearity involving k sources exists, then only a maximum of n-k sources need be included in CMB calculations, and 2^{n-k}-1 regressions need be calculated. With the Quail Roost II data set, for example, several of the 13 sources had strong collinear relationships and four or five fewer sources need be included in any CMB model.

The APR procedure is demonstrated using a synthetic data set created for the Philadelphia area. Synthetic data sets have the advantage that complete control is maintained over the data: the "true" apportionment and the errors are known. However, the error structure and composition of the synthetic data sets may not be realistic. The synthetic data set created here was designed only to illustrate the diagnostic procedures. The data set was constructed using the PEM dispersion model, source inventory and meteorology from Philadelphia (Section 3) and the same procedure used in Quail Roost II. In brief, the 13 profiles from Quail Roost II were assigned to the 12 source classes used in PEM modeling, multiplied by their predicted contributions to receptor concentrations, and contaminated with random errors. The synthetic data set used for this evaluation was derived from period 2 meteorology at receptor 10 (see Section 4), and had major contributions from three sources. Soil: 50.72 ug/m^3; wood: 19.74 ug/m^3; and automobile: 7.80 ug/m^3. It also included minor contributions from

other sources, as shown in Table 19. Ordinary least squares with 8 profiles and a constant were used in a simple CMB approach. Four profiles, as indicated in the collinearity analysis, were eliminated from the CMB model.

Mallow's C_p statistic, which is related to the mean square error of the estimated source contribution, was the criterion used for source selection in the APR procedure (Table 18). For p sources included in a model (p ranging from 1 to 13), the five best models were generated. For example, the best one variable model used Coal-A; the second best used Oil-B, (sources 6 and 5 respectively). The best two variable models used soil and wood sources (sources 10 and 12). In general, models with low values of C_p are of interest. This corresponds to a 9 variable model. However, Table 18 shows that a number of models with various combinations and numbers of variables have about the same fit, i.e., there may be no clearly superior model. The Table also shows that the models selected tend to be quite similar, i.e., include or exclude similar sources. Interesting, while all models composed of five or more sources included the major contributing sources of the synthetic data set (sources 10, 11, and 12), models of fewer variables may not include these sources. Models with a large number of sources tended to include sources that were identified as being collinear, e.g., coal-A and aggregate (sources 6 and 7). This indicates that a model with fewer than 9 variables may be preferable since collinear source profiles will not be accurately estimated.

Since the all possible regressions procedure tests all combinations of sources it may be more comprehensive than the procedure used in Quail Roost II. However, unlike the Quail Roost II procedure, it does not focus on removing negative source contributions. This may not be a serious drawback since the procedure generates many "near optimum" models. If the 2nd or 3rd best model of p sources contains negative source estimates, then models containing p-1 sources may be examined. The likelihood of significant and negative source estimates should decrease as models contain fewer sources.

Influential Characteristics

Influential characteristics (or observations) are filter characteristics that exert a disproportionate influence on the fitted model. For example, lead is an influential characteristic for automobiles,

REGRESSIONS WITH 1 VARIABLES (CP)

CRITERION	VARIABLES
109293.	6
113790.	5
116458.	10
125723.	12
142717.	11

REGRESSIONS WITH 2 VARIABLES (CP)

CRITERION	VARIABLES
1390.26	10 12
7533.54	6 12
13928.	6 11
49429.3	5 6
50748.8	2 6

REGRESSIONS WITH 3 VARIABLES (CP)

CRITERION	VARIABLES
711.606	6 10 12
1094.24	10 11 12
3933.7	6 7 12
5038.32	6 9 12
5745.85	4 6 12

REGRESSIONS WITH 4 VARIABLES (CP)

CRITERION	VARIABLES
446.823	6 10 11 12
485.597	6 10 12 13
511.658	6 9 10 12
519.943	1 6 10 12
552.521	2 6 10 12

REGRESSIONS WITH 5 VARIABLES (CP)

CRITERION	VARIABLES
61.0221	5 10 11 12 13
243.687	6 9 10 11 12
272.088	6 10 11 12 13
296.008	1 6 10 11 12
341.835	2 6 10 11 12

REGRESSIONS WITH 6 VARIABLES (CP)

CRITERION	VARIABLES
52.6796	5 6 10 11 12 13
62.2877	4 5 10 11 12 13
62.7126	5 7 10 11 12 13
135.011	6 9 10 11 12 13
173.831	4 6 9 10 11 12

REGRESSIONS WITH 7 VARIABLES (CP)

CRITERION	VARIABLES
25.4399	2 4 5 10 11 12 13
27.2665	3 6 9 10 11 12 13
28.0219	5 6 9 10 11 12 13
49.3224	4 5 6 10 11 12 13
91.4441	6 8 9 10 11 12 13

REGRESSIONS WITH 8 VARIABLES (CP)

CRITERION	VARIABLES
7.75109	4 5 6 7 10 11 12 13
7.86788	3 4 6 7 10 11 12 13
11.6995	2 4 5 6 10 11 12 13
11.9773	1 4 5 6 10 11 12 13
13.9464	1 2 4 5 10 11 12 13

REGRESSIONS WITH 9 VARIABLES (CP)

CRITERION	VARIABLES
6.64801	2 4 5 6 7 10 11 12 13
6.99988	1 4 5 6 7 10 11 12 13
8.83725	3 4 5 6 7 10 11 12 13
9.32423	3 4 6 7 9 10 11 12 13
9.39112	4 5 6 7 8 10 11 12 13

REGRESSIONS WITH 10 VARIABLES (CP)

CRITERION	VARIABLES
8.11824	1 2 4 5 6 7 10 11 12 13
8.29817	2 3 4 5 6 7 10 11 12 13
8.43179	2 4 5 6 7 9 10 11 12 13
8.61388	2 4 5 6 7 8 10 11 12 13
8.66667	1 3 4 5 6 7 10 11 12 13

REGRESSIONS WITH 11 VARIABLES (CP)

CRITERION	VARIABLES
10.026	1 2 3 4 5 6 7 10 11 12 13
10.2101	2 4 5 6 7 8 9 10 11 12 13
10.2512	2 3 4 5 6 7 9 10 11 12 13
10.3361	1 4 5 6 7 8 9 10 11 12 13
10.5527	1 3 4 5 6 7 9 10 11 12 13

REGRESSIONS WITH 12 VARIABLES (CP)

CRITERION	VARIABLES
12.0252	1 2 3 4 5 6 7 9 10 11 12 13
12.026	1 2 3 4 5 6 7 8 10 11 12 13
12.1117	1 2 4 5 6 7 8 9 10 11 12 13
12.1339	2 3 4 5 6 7 8 9 10 11 12 13
12.2808	1 3 4 5 6 7 8 9 10 11 12 13

REGRESSIONS WITH 13 VARIABLES (CP)

CRITERION	VARIABLES
14.	1 2 3 4 5 6 7 8 9 10 11 12 13

Table 18. Results of all possible regression procedure using synthetic data set and Mallow's C_p statistic. Table 17 shows the identification of the sources (shown under variables).

since the estimated automobile contribution is roughly proportional to the measured lead concentration, which is a fairly unique tracer for this source. In general, estimated source contributions may depend more on the influential points than the rest of the data.

Influential characteristics may increase the accuracy and decrease the uncertainty of the estimate of the source contribution if the characteristics are correct. Such (legitimate) extreme characteristics are useful as indicators of a particular sources in RM, and also serve to show which elements or characteristics should be analyzed in the filter sample. However, the source apportionment estimate may be misleading if the influential characteristics result from improperly recorded data, measurement errors, or inappropriate source profiles.

Many diagnostic procedures exist to detect influential characteristics. These procedures may be classified into three general families (Belsley, et. al. 1980):

1. Single and multiple row deletions: Essentially, one or more filter characteristics is removed from the analysis, and the source apportionment is re-estimated. Large changes between the source apportionment estimated with missing characteristics and with the complete set of characteristics may indicate critical (i.e., possibly unique) filter characteristics and possibly uncertain source estimates. This process is repeated for each filter characteristic. Single and multiple row deletion measures include:

change of estimated source class coefficients---DFBETA(S)

change of fit--DFFIT(S), PRESS

2. Examination of the source profile (X) matrix: These measures examine only the source profile matrix and look for single or multiple characteristics which are unique to each profile. If few characteristics distinguish a profile, the source apportionment may be sensitive to these characteristics. Common measures include:

diagonals of the projection matrix $H = X(X^TX)^{-1}X^T$

covariance matrix--COVRATIO

3. Examination of residuals: Residuals (the difference between observed and fitted filter characteristics in CMB models) may be examined to

determine if least squares procedures are appropriate and tests of significance are valid, i.e., by examining whether the residuals are correlated and normally distributed. In addition, plots of residuals may provide a great deal of information concerning influential points. Residual diagnostics include:

normal probability plots
standardized and studentized residuals
partial residual plots
partial regression leverage plots

Two types of diagnostics are illustrated using the synthetic data set and ordinary least squares procedures. Five of the profiles that showed collinearity problems were removed from the model. Actual and estimated source contributions are shown in Table 19. This apportionment is meant only to illustrate the use of diagnostics: no attempts were made to improve the apportionment, e.g., by omitting sources with negative contributions.

DFBETAS are single row deletion statistics, which quantify the effect of an individual filter characteristic on the estimated source class contribution. DFBETAS indicate the change of the estimated source contribution in terms of its standard error. A reasonable cut-off for determining influential characteristics is $\pm$ 1, where omitting a characteristic, e.g., Vn concentration, might change the estimated source contribution by one standard deviation (of its uncertainty).

Table 20 shows DFBETAS for the synthetic data set. Each row of the Table shows the DFBETAS for the removal of one characteristic from the CMB model. For example, removing characteristic 1, the mass of carbon, from the regression would change the estimated oil-A contribution by 3.83 times the standard error of this coefficient, a large amount. Five characteristics (1=C, 3=AL, 7=K, 13=Fe, and 19=Pb) have DFBETAS which exceed the cut-off for a several source classes. As expected, Pb is an influential characteristic for the auto source class. The four other influential characteristics affect steel-B, oil-A, incinerator, aggregate, coal-A, soil, coal-B and wood classes.

Partial residual plots permit a visual indication of influential subsets. Each plot reveals the relationship between particular source profiles, adjusted for its collinearity with the other profiles, and the

-Source Class-	Source Apportionment in ug/m^3 -Actual--	-OLS Estimate-	-Robust Estimate-
Steela	0.016		
Steelb	0.000		
Oila	0.121	3.6	3.6
Incin	0.009	-1.0	-1.0
Oilb	0.275		
Coala	0.022	13.7	13.8
Aggreg	0.021	-9.6	-9.7
Glass	0.076		
Basalt	0.019		
Soil	50.321	44.0	44.1
Auto	7.795	4.7	4.7
Wood	19.737	20.7	20.6
Coalb	0.000	-6.4	-6.5

Table 19. Estimated CMB source apportionment using 8 source classes and synthetic data set; actual apportionments are PEM predictions; only coefficients with 95 percent confidence are shown.

OBSER.	STEELB	OILA	INCIN	COALA	AGGREG	SOIL	AUTO	WOOD	COALB	CONST
1	1.170	3.831	-3.258	-0.545	-0.539	1.686	0.219	43.510	-3.015	-0.315
2	0.026	0.066	0.136	0.001	-0.023	0.066	0.314	-0.208	-0.108	-0.010
3	0.938	1.867	0.122	-0.117	0.192	-0.346	-0.171	-0.169	-2.517	-0.198
4	0.039	-0.422	0.096	-0.197	0.111	-0.314	0.087	0.145	0.729	0.070
5	0.021	-0.514	0.003	0.055	-0.037	0.213	0.029	-0.055	-0.439	0.016
6	0.453	-0.346	0.089	0.538	-0.551	0.434	-0.190	-0.416	-0.223	-0.207
7	1.597	-0.557	2.369	1.797	-1.878	1.322	0.010	-1.742	-0.437	-0.659
8	-0.155	-1.555	-0.728	0.447	0.287	-1.620	0.029	0.198	1.472	0.075
9	0.045	-0.061	-0.159	0.130	-0.142	0.117	-0.136	-0.044	-0.073	0.236
10	0.155	-0.201	-0.027	0.175	-0.140	0.041	0.141	-0.206	0.097	-0.440
11	0.002	-0.001	0.002	0.001	-0.001	-0.000	0.004	-0.003	0.002	-0.010
12	0.012	0.014	-0.019	0.003	-0.010	0.018	-0.030	0.004	-0.030	0.062
13	3.222	2.354	1.114	-1.834	0.982	1.090	0.275	-0.410	-1.702	-0.485
14	0.042	-0.056	0.011	0.043	-0.031	0.004	0.064	-0.063	0.041	-0.175
15	0.017	0.004	0.047	-0.015	0.016	-0.009	0.065	-0.025	0.026	-0.145
16	-0.506	0.163	0.426	-0.507	0.545	-0.441	0.241	0.406	0.331	-0.159
17	-0.007	0.003	-0.003	-0.004	0.004	-0.002	-0.009	0.009	-0.002	0.024
18	-0.631	0.227	0.060	-0.504	0.502	-0.353	0.603	0.158	0.056	1.065
19	0.086	0.313	0.207	-0.051	-0.012	0.104	-3.850	1.136	-0.238	0.312

Table 20. DFBETAS row deletion statistics for CMB of synthetic data set. Observations refer to the elemental measures in Table 13.

residuals (the difference between fitted and observed filter characteristics), adjusted for the other sources (i.e., the source contributions of the other sources have been removed from the residuals). Thus, each plot illustrates the fit between source profiles and filter characteristics where the effect of the other sources has been removed.

Partial residual plots for 8 source classes in the CMB model using the synthetic data set are shown in Figure 14. For example, the top left plot is the partial residual plot for the soil class. The estimated soil contribution is related to the slope of the regression line (shown with asterisks); the significance or fit of the data to the soil profile is indicated by the scatter around the regression line. The plot for the incinerator class shows a negative slope (and thus negative source estimate) and considerable scatter, both of which imply that results for this source may not be meaningful.

Influential points or subsets typically form isolated clusters of point(s) located some distance from the majority of points on the partial residual plots. Influential points heavily influence the regression line, i.e., the source estimate, since the regression line minimizes the sum of squared differences. For example, point D (indicated with an arrow) (characteristic 7=K) is an influential point for the oil-A, incinerator, coal-A, aggregate and soil classes. This point alone heavily weights the regression line for oil-A, incinerator, coal-A and aggregate source classes, which were poorly estimated by OLS. The validity of the K measurement is thus highly important for these source estimates. Similarly, point K (19=Pb) is influential for the auto and wood sources. Error in the lead measurement will highly bias the auto estimate. However, the wood source estimate may be more resistant since other characteristics lie on the regression line. This information is similar to that provided by the DFBETAS. The partial regression plots also show an influential subset--not definitively indicated by the DFBETAS--in the case of coal-B, which has two influential points, B (3=Al) and D (7=K).

DFBETAS and partial residual plots may be effective ways to determine the effect of both single and multiple influential characteristics in CMB models. Influential characteristics may require further analysis to determine the legitimacy of the characteristics.

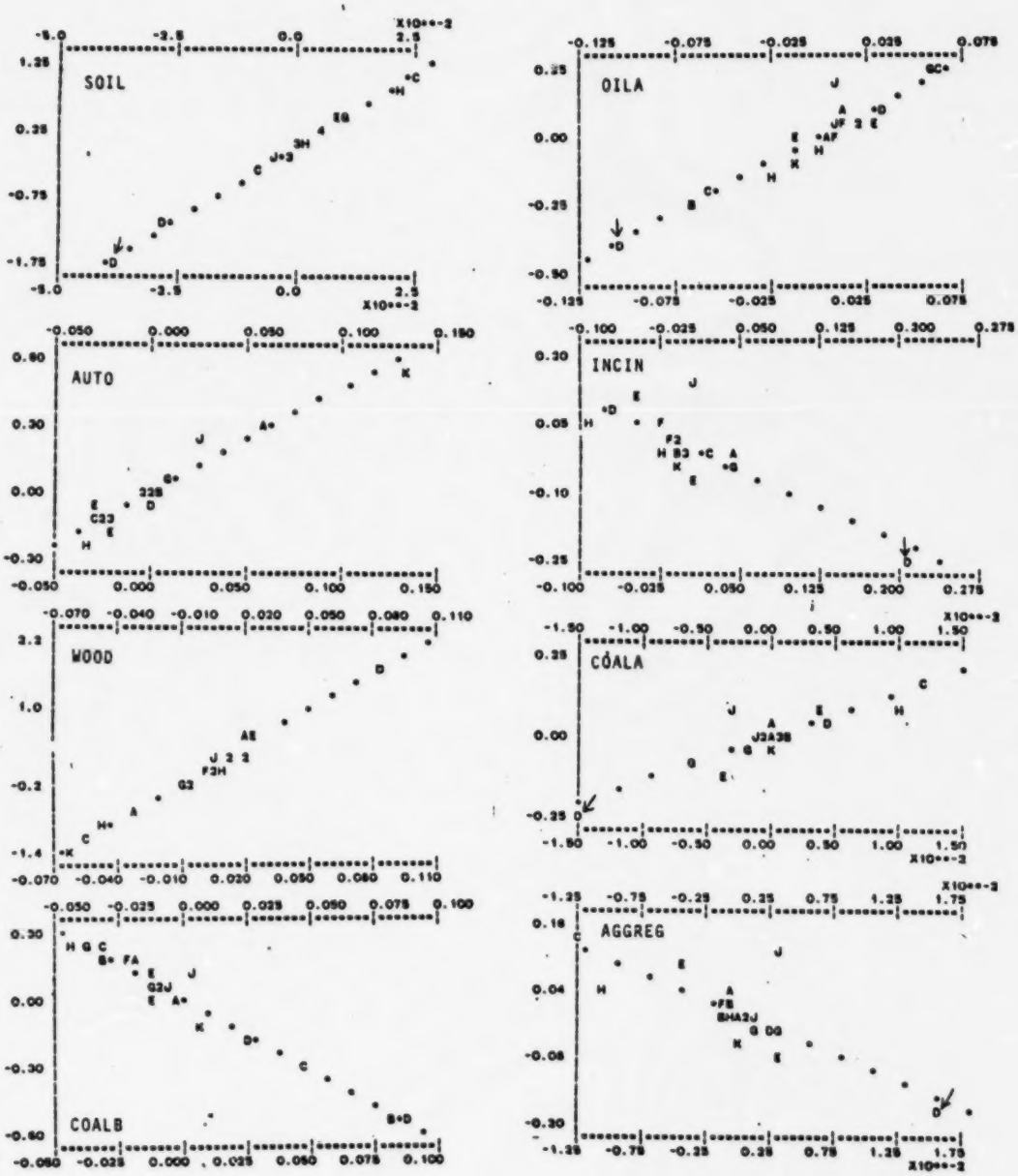

Figure 14. Partial regression plots for 8 source classes. Adjusted elemental mass on ordinate; adjusted source profile (as indicated) on abscissa. Fitted least squares line is shown with asterisks.

Robust Regression

Robust regression procedures are designed to diminish the effect of outliers, such as erroneously measured filter characteristics, data entry mistakes, etc. In ordinary least squares (OLS), outliers tend to have a disproportionate effect on estimated source contributions. In robust regression, the influence of outliers is constrained by downweighting outliers. Robust procedures are especially useful when the normality assumptions of OLS are in question. The principal value of robust regression in CMB RM, perhaps, is to provide a check on OLS results. Agreement between the OLS and robust regression results may help insure that the estimated source class contributions are meaningful. Robust regression may be viewed as an automated way of determining the influence of outliers (as well as influential points).

Most robust procedures employ iteratively reweighted least squares. First, source estimates and residuals are calculated using ordinary OLS. Then, a specified influence function (Hampel, 1974) is used to downweight large residuals in a weighted least squares regression. An iterative process using weighted residuals and the influence function continues until convergence. Watson's "effective variance" procedure also uses iteratively reweighted least squares procedures. However, the effective variance procedure gives more weight to ambient source measurements which are measured with precision, as well as source class estimates which are certain. It does not diminish the effect of outliers which tend to pull the OLS solution.

Robust procedures were used on the synthetic data sets using 8 source signatures in TROLL. The standard convex Huber influence function was used to weight the squared residuals (Peters, et. al., 1981). Robust results were very similar to OLS results, i.e, few characteristics were significantly downweighted (Table 19). This probably occurred because the contamination method did not generate outliers (only normal errors were used.) In practice, however, results using OLS and robust procedures may vary.

It is also possible to determine which characteristics were downweighted in the robust regression. Examination of such points may identify possible errors. We note that it is possible to combine robust

procedures with ridge regression and the effective variance technique. Lastly, a procedure similar to robust regression, called bounded-influence regression, designed to limit the bias caused by contamination of data such as that caused by keypunch mistakes (Peters, et. al., 1981), may have application to CMB apportionments.

HYBRID RECEPTOR/DISPERSION MODELS

This section discusses several possibilities for hybrid dispersion/receptor models. Hybrid models use a receptor model approach in conjunction with source emission rates, source locations and/or dispersion information. Such models conceivably might provide a more accurate and flexible means of source apportionment. They may also help reconcile differences between source and receptor models.

Some potential uses of hybrid RM/DM approaches include:

Operational validation. Receptor and dispersion models are used separately. Inter-model comparisons may help identify emission inventory deficiencies, i.e., missing or mis-estimated emission sources. Inter-comparisons can help "confirm" apportionment estimates by employing a "consensus" standard.

Diagnostic validation. Model comparisons are used to refine and calibrate model parameters, e.g., dispersion coefficients and source profiles. Such validation may be appropriate for model development.

Complementary use. Outputs from receptor and dispersion models are combined. For example, DM might be used to apportion regional or background concentrations, and RM might estimate local concentrations. Other examples include using RM with filter samples collected according to the observed frequency of meteorological conditions, to determine long term averages; collecting filter samples during meteorological patterns which result in the highest DM predictions; restricting the profiles in CMB models to upwind sources; and calculating back-trajectories which incorporate transformation and deposition for receptor determined mass source apportionments (e.g., Thurston, 1983). Some of these approaches may be more practical with short-term (e.g., hourly) filter samples.

Coupled models. All data, including meteorology, source emissions and profiles and filter characteristics are used in coupled models. Coupled models intimately combine receptor and dispersion approaches, and thus may be more complicated than other hybrid approaches.

Coupled models might be classified by their primary orientation, around either dispersion or receptor approaches. Some speculations concerning possible coupled hybrid dispersion/receptor models are given below.

For receptor oriented hybrid models, outputs of DMs might be treated stochastically. CMB receptor models might then be extended by either including DM predictions as priors in Bayesian optimizations, or by using DM predictions of source contributions as coefficient weights in weighted optimizations. Analogous methods are possible for multivariate RMs. Here, preprocessed meteorological data might become new variables in a factor analysis or multiple regression model. Association of particular meteorological patterns with source class signatures may identify the likely direction and distance of contributing sources. Alternately, source contributions predicted by DMs may become variables in factor analyses, along with the usual filter characteristics. Associations of predicted source contributions with the respective source profiles may indicate areas of agreement between the models.

The second general type of coupled models is based around dispersion modeling. In some ways, this approach is similar to the diagnostic validation discussed earlier applied to DMs. The (deterministic) inputs or parameters of DMs are considered as stochastic variables (with estimated distributions). Optimization is used to match DM predictions to observed concentrations or receptor determined apportionments, at the same time maximizing the probability of the stochastic variables in the DM. Yamartino (1982) and Cooper (1982) have used a time series of observed concentrations to estimate average source strength by region and sector, respectively. The identification of large emissions in areas without known sources may help quantify the regional (background) contribution. These studies did not use aerosol characteristics.

More sophisticated coupled models may be possible if short-term (CMB) receptor model results are available and of suitable accuracy. This may

permit the estimation of short-term parameters in dispersion models. For example, source inventories generally include only annual average emission rates. However, hourly and seasonal emission rates are highly variable. The distribution of hourly emissions may be estimated. The optimization model may be used to select emission rates, within the assigned distribution, that produce results closest to the source apportionment determined previously using RMs. DM using the revised emission rates then might provide the hybrid source apportionment. Similar approaches may be possible for other variables in dispersion models, e.g., dispersion coefficients and wind direction.

There has been relatively little work in the development of hybrid models. Some of these models may be used to help apportion both local and regional pollutants in the Philadelphia study. Data from this study, as well as from realistic synthetic data sets, may provide a means to test the feasibility of the various hybrid models.

COMPARISONS BETWEEN SOURCE AND RECEPTOR MODELS

Some aspects of model validation and model inter-comparisons are discussed in this section with reference to the Philadelphia study. The evaluation of similarities and differences between dispersion and receptor models may help explain strengths and weaknesses of the models, and possibly indicate the certainty of the source apportionment.

One approach for identifying and quantifying the likely causes of model agreement (or discrepancy) might use regression or factor analyses. These procedures may be used to associate measures of agreement between RM and DM results with meteorological data, averaging time, source class, and other information.

Evaluation Criteria

This section addresses the quantitative "performance" measures used to evaluate model results. In the Philadelphia study, both RM and DM results will be compared, and the true source apportionment is not known. Such inter-model comparisons involve somewhat different concerns than model validation studies where predicted concentrations are compared to observed concentrations, or the Quail Roost exercise, which inter-compared only receptor models.

There are several useful strategies for inter-model comparisons:

(1) Comparison between all models. Provides the most information and makes the fewest assumptions, but (n-1)! comparisons must be made for n models, a potentially large number.

(2) Comparison of each model's results to the mean or median result. This is useful since it highlights deviations from the mean or median prediction. However, there is no assurance that the mean or median prediction is the best estimate of source apportionment.

(3) Comparison to an estimate of true source apportionment, based on considering and weighing all available evidence. Joint and independent application of RM and DM as suggested by Core, et.al., (1982) might be the

means to obtain the source apportionment estimate. Additional ways of combining receptor and source models were discussed previously.

While the first two strategies permit direct comparisons of model results, it is felt that the third strategy may be the most comprehensive approach to model inter-comparison. However, as discussed previously under the section on hybrid receptor/dispersion modeling, there are not yet objective and practical approaches which appropriately combine all evidence.

A second issue of RM and DM comparisons concerns the quantity compared. In general, it would seem that the quantities compared should relate to modeling objectives. Comparison of (possibly size fractionated) source class contributions of the particulate mass might be appropriate, as used in Quail Roost II. It is important to realize that neither DMs nor RMs apportion regional sulfate, which may contribute much of the fine particulate mass. DMs, such as PEM, do not model regional sources (beyond 60 km distance). RMs may not accurately apportion sulfate since sulfate does not have identifiable tracers. Consequently, apportionment of the sulfate in the Philadelphia study will involve large uncertainties. Apportionment of sulfate might be broken out separately from the apportionment of local sources, to help clarify the contribution from regional sources.

Third, the different nature of the outputs produced by DM and RM should be recognized in inter-comparisons. DMs provide deterministic point estimates; RMs provide statistical or qualitative estimates. While it is possible to weight comparisons between RM results with estimates of their statistical confidence, this can not be accomplished easily with DM. One possible solution is to compare only the statistically significant RM results to DM results. Statistically insignificant results might be set to zero. One or several confidence levels might be selected for this purpose. (Confidence intervals should be explicity incorporated in the calculation of the best estimate of source apportionment, as discussed later.)

Averaging Time

Bias, distributional effects and extrapolation errors are three effects associated with averaging time which may influence model inter-comparisons.

DMs usually can predict long-term, i.e., seasonal and annual,

concentrations with greater accuracy than short-term, i.e, hourly to daily, concentrations. Many of the errors of short-term DMs result from inaccurate or incomplete data from the source inventory, meteorology and ambient monitoring. Many of these short-term errors are random, and tend to be averaged out in long-term concentration averages. (These generalizations may not apply to the modeling of regional pollutants.)

RMs also may be susceptible to short-term errors since source class profiles are usually assumed to be time and source averages of measured or estimated profiles. The errors in the source profile may be small if many individual emission sources compose a source class (and if there are no systematic biases). For example, if in a particular source class there are n individual sources which equally contribute to observed concentrations, then the uncertainties of the source profile may be expressed as:

$$\text{Standard deviation of profile} = \frac{\text{standard deviation of individual profiles}}{\sqrt{n}}$$

since variances are additive. This suggests that source profile errors will be small for source classes composed of many sources, even in short time periods. Thus, the accuracy of RM based apportionments of automotive, oil, soil, etc., source classes may be largely insensitive to averaging time. In contrast, the accuracy of apportionments for some source classes composed of only a few sources may be more sensitive to averaging time. Thus, long-term apportionments from both RMs and DMs may be the most valid, although some short-term RM results may be equally valid. This may be tested by contrasting measures of agreement between RM and DM results for different source classes at different averaging times.

It may be worthwhile to evaluate model agreement in short time periods since, in many circumstances, it may not be possible to sample and analyze a large number of samples. This might exclude multivariate models, since these models require many observations. However, such comparisons may yield information of practical value regarding the accuracy and reliability of CMB models. (The Quail Roost II exercise primarily used multivariate models, and thus only the average apportionment over 40 12-hour averaging periods was evaluated.)

The confidence level or uncertainty in short-term (and long-term) source apportionments should be included in inter-model analyses. The uncertainty of single and multiple short-term apportionments, e.g., by

applications of CMB models, might be estimated using statistics such as the mean coefficient of variation of estimated contributions in particular source categories.

The second effect of averaging time is its influence on pollutant distributions. It is widely recognized that pollutant concentrations at short averaging times have approximately lognormal distributions and large standard deviations. Concentrations at long averaging times have much smaller standard deviations. Similarly, the standard deviation of source apportionments will depend on averaging time. Comparisons between DM and RM should account for the these distributions by employing appropriate performance measures, as discussed by the AMS (1979) and Fox (1981). This also suggests that hybrid RM-DM or RM models which use short averaging times (e.g., several hours) may be subject to non-normal errors. Consequently, such models should employ robust procedures which are resistant to such "contaminated" data, such as robust regression discussed earlier.

The third effect of averaging time concerns extrapolation errors. In general, seasonal or annual source apportionments using RM and (necessarily) a limited number of filters will require extrapolation of data. The number of filter samples required to produce representative longer term source apportionments is unknown, but is likely to be dependent on the site and circumstance.

RECEPTOR MODEL PROTOCOLS

Pace (1983) has discussed possible roles for receptor models in the regulatory framework. There are a number of important and unresolved questions concerning the practical use of receptor models in the regulatory setting. Protocols represent well defined and justified methods which help assure quality results. Protocols for receptor models may be classified into three areas: 1) protocols for the physical aspects of the study, including the design, siting, operation, and quality control and assurance of monitoring and filter analyses; 2) modeling protocols, which include model selection, treatment of uncertainty and diagnostics; and 3) protocols for model inter-comparisons, to determined preferred approaches. This section discusses aspects of RM protocols using this classification.

Protocols for Monitoring and Analysis

There are a number of general issues related to the amount and quality of the information required in RM studies. These are important issues since most costs of RMs are associated with sampling and analysis of filters, rather than modeling. These issues and trade-offs include:

(1) Number of analytic tests on the filter samples: There is almost an unlimited amount of analytical testing that can be done on a set of samples. Obviously, it is important to arrange testing such that the most cost effective methods are conducted first. Analytical tests that can break collinear relationships between sources can be determined by collinearity diagnostics. Site-specific cut-offs for analyses might be established, beyond which further analysis is not cost-effective. This trade-off between more and fewer analytical tests could be defined prior to regulatory use.

(2) Number of samples: A minimum number of filter samples is required for representativeness; a larger number of samples is required for multivariate receptor approaches. Here again it may not be worthwhile to collect additional samples. Documentation of RM performance for specific sites and situations might help define the necessary number of samples.

(3) Source sampling: More extensive source sampling may increase the accuracy and selectivity of RM. Such analysis is expensive, time consuming, and may not yield representative signatures. Thus, as in filter analysis, the costs of source sampling can be balanced against its decreasing marginal value.

(4) Length of sampling period: At this point most sampling periods are 12 hours in length. This allows a representative sample of seasonal conditions with a reasonable number of filters. However, 12 hour intervals make it difficult to use the information contained in wind direction and other meteorological data. It is now possible to obtain hourly samples with sufficient loadings for the analytical procedures. With hourly samples, the source apportionment problem might well decompose into different problems for each wind direction and thus yield finer source resolution. The cost,

however, of running 20 to 25 days of hourly samples through the analytical procedures would be prohibitive. Thus, a trade-off exists between the representativeness of the data and the ability to utilize meteorological information.

Modeling Protocols

The diagnostic procedures discussed previously are a subset of modeling protocol issues. The main objectives of using diagnostic tools are to increase the speed and effectiveness of receptor modeling and to decrease the chance of spurious results. Diagnostics might be incorporated into model protocols to 1) detect the presence of problems such as collinearity, outliers and influential observations, 2) assess the extent to which the source apportionment is degraded, and 3) determine whether corrective action is necessary. The usefulness of the various diagnostic procedures might be subject to the same sort of evaluation as model comparison, in order to determine which procedures are the most appropriate.

A receptor modeling protocol, which incorporates diagnostics, might include:

1. Use of source inventory, dispersion modeling, factor analysis, or microscopy to identify major source contributors.

2. Use of measured or estimated source profiles in an effective variance CMB or multivariate analysis to quantify impacts and possibly detect additional sources.

3. Estimate the effect of collinearity in the source profiles (e.g., using singular value decomposition).

   If necessary, re-estimate apportionment (e.g., using ridge or principal components regression, or deletion/combination of source classes using all possible regressions). Obtain positive and significant source contributions.

4. Determination of the sensitivity to outliers and influential points using DFBETAS, partial residual plots, and/or effective variance techniques.

5. Confirm CMB results using robust regression techniques, or "fresh" data.

Clearly, receptor model protocols will depend on the circumstances and the effort of the study.

Protocols for Inter-comparison of Receptor Models

Model inter-comparison serves the purposes of documenting model performance and uncertainty, and determining model applicability, i.e., matching models and uses. Inter-comparison studies of receptor models have not stressed both objectives, largely due to limited data. Model inter-comparisons may include measures of model adequacy for different source and background compositions (e.g., rural western vs. urban eastern sites); varying averaging times; and various levels of study effort (e.g., with or without source sampling). More effort is needed to estimate confidence levels which are representative.

SUMMARY

Some of the major issues in the use of receptor models are:

(1) Art versus science in the application of RM. Currently there is a substantial amount of imposed "intelligence" that is introduced into RM procedures by experienced practitioners. Present RM studies are generally custom designed, including selection of source signatures, filters and analysis. In the regulatory context, some of the discretionary elements of RM might have to be removed to reduce the chances for misuses of the models. Regulatory protocols must balance the need to ensure robust and representative results with the interpretative and case-specific nature of RMs. A middle ground might ensure that monitoring, filter analysis, quality assurance and control procedures are adequate, and RM results are not

spurious. Also, appropriate measures of uncertainty must be included.

(2) Development of representative source profiles and synthetic data sets. The variation in source profiles (over time and space) and the deviation from the RM assumptions can be determined from source or near field measurements, or perhaps derived using wind trajectory analysis. Synthetic data sets with realistic error structures and compositions for various aerosol regimes, e.g., rural western vs. urban eastern, may be used to construct RM protocols. Such data sets may help identify the resolution and uncertainties of the various receptor models as well as the necessary study effort (sampling and analysis). Inter-model comparisons using this data can be used to select preferred models and diagnostic approaches.

(3) Hybrid receptor/dispersion approaches. Hybrid models require more data than either approach alone. Such models may be cost-effective if source inventories and meteorological data are available. If hybrid models permit significantly improved performance in terms of accuracy and flexibility of source apportionment, their expense and complexity may be justified in other circumstances. At present, hybrid models have not been demonstrated and critically evaluated.

REFERENCES

Air Pollution Control Association (1982): Specialty Conference on Receptor Models Applied to Contemporary Pollution Problems. Danvers, MA, APCA Publication. 388 pp.

Cooper, D.W., Receptor-Oriented Source-Receptor Analysis. loc. cit.

DeCesar, R., Evaluation of Multivariate and Chemical Mass Balance Approaches to Aerosol Source Apportionment using Synthetic Data and an Expanded Pacs Data Set. loc. cit.

Yamartino, R.Y., Formulation and Application of a Hybrid Source-Receptor Model. loc. cit.

American Meteorological Society (1979): Air Quality Modeling and the Clean Air Act: Recommendations to EPA on Dispersion Modeling for Regulatory Applications. Boston, MA. 268 pp.

Belsley, D.A., E. Kuh, R.E. Welsch (1980): Regression Diagnostics: Identifying Influential Data and Sources of Collinearity. John Wiley and Sons, New York.

Cooper, Y.A., J.G. Watson: Receptor Oriented Methods of Air Particulate Source Apportionment. J. Air Poll. Control Assoc. 30 1116-1125.

Core, J.E. et. al. (1982): Particulate Dispersion Model Evaluation: A New Approach Using Receptor Models. J. Air Pol. Control Assoc. 32 1143-1147.

Energy Information Administration (1980): Thermal Electric Power Plant Construction and Annual Production Expenses. Washington, D.C.

Environmental Research and Technology, Inc. (1981): The State of the Art of Receptor Models Relating Ambient Suspended Particulate Matter to Sources. Report P-A422 to US Environmental Protection Agency, Research Triangle Park, NC.

Fox, D.G. (1981): Judging Air Quality Model Performance, Review of the Woods Hole Workshop. American Meteorological Society, Boston, MA.

Hampel, F.R. (1974): The Influence Curve and its Role in Robust Estimation. J. Amer. Statist. Assoc. 69 383-394.

Huber, P.J. (1981): Robust Statistics. John Wiley and Sons, New York.

Information Processing Center (1980): TROLL Users Guide. Massachusetts Institute of Technology, Cambridge, MA.

Montgomery, D, E.A. Peck (1982): Introduction to Linear Regression Analysis. John Wiley and Sons, New York.

National Academy of Science, (1983): Acid Deposition: Atmospheric Processes in Eastern North America. National Academy Press, Washington, D.C. 275pp.

Pace, T.G. (1983): Models to Develop Controls Strategies for PM-10, in Proceedings of the 76th Annual Meeting of the Air Pollution Control Assn. Atlanta, GA, June 19-24.

PEDCo Environmental (1979): TSP Source Inventory Around Monitoring Sites in Selected Urban Areas, Philadelphia. Report to US Environmental Protection Agency, Monitoring and Data Analysis Division, Research Triangle Park, NC. 92 pp.

Rao, Shankar K. (1983): Plume Concentration Algorithms with Deposition, Sedimentation and Chemical Transformation IAG-AD-13-F-1-707-0. National Oceanographic and Atmospheric Administration, Oak Ridge, TN. 87 pp.

Sehmel, George (1980): Particle and Gas Dry Deposition: A Review. Atmos. Environ. 14 983-1011

Suggs, J.C., R.M. Burton (1983): Spatial Characteristics of Inhalable Particles in the Philadelphia Metropolitan Area. J. Air Pol. Control Assoc., 33 686-91.

Texas Air Control Board (1979): Texas Episodic Model, User's Guide PB80-227572. National Technical Information Service, Springfield, VA.

Thurston, G.D. (1983): A Source Apportionment of Particulate Air Pollution In Metropolitan Boston. Ph.D. Thesis, Harvard School of Public Health, Boston, MA.